

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	0	7,7-diphenyl-2,4,6-heptatrienoic	USPAT; EPO; JPO; DERWENT	OR	OFF	2004/11/19 12:09
L2	0	(Histone adj deacetylase) and (("562/495").CCLS.)	USPAT; EPO; JPO; DERWENT	OR	OFF	2004/11/19 12:09
L3	0	("I7andI17").PN.	USPAT; USOCR; EPO; JPO; DERWENT	OR	OFF	2004/11/19 12:09
L4	0	heptatrieno\$ and (("562/491").CCLS.)	USPAT; EPO; JPO; DERWENT	OR	OFF	2004/11/19 12:09
L5	0	heptatrien\$ and (("562/491").CCLS.)	USPAT; EPO; JPO; DERWENT	OR	OFF	2004/11/19 12:09
L6	0	(dodecen\$ and insecticid\$) and "2005271"	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2004/11/19 12:09
L7	279	(514/559).CCLS.	USPAT; USOCR; EPO; JPO; DERWENT	OR	OFF	2004/11/19 12:09
L8	885	(514/562).CCLS.	USPAT; USOCR; EPO; JPO; DERWENT	OR	OFF	2004/11/19 12:09
L9	414	(514/564).CCLS.	USPAT; USOCR; EPO; JPO; DERWENT	OR	OFF	2004/11/19 12:09
L10	716	(514/570).CCLS.	USPAT; USOCR; EPO; JPO; DERWENT	OR	OFF	2004/11/19 12:09
L11	179	(514/571).CCLS.	USPAT; USOCR; EPO; JPO; DERWENT	OR	OFF	2004/11/19 12:09
L12	2	"53101527".pn.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2004/11/19 12:09
L13	456	Histone adj deacetylase	USPAT; EPO; JPO; DERWENT	OR	OFF	2004/11/19 12:09

L14	5855	hydroxamic	USPAT; EPO; JPO; DERWENT	OR	OFF	2004/11/19 12:09
L15	3694	histone	USPAT; EPO; JPO; DERWENT	OR	OFF	2004/11/19 12:09
L16	1	heptatrienoic and histone	USPAT; EPO; JPO; DERWENT	OR	OFF	2004/11/19 12:09
L17	1	7-phenyl-2,4,6-heptatrienoic	USPAT; EPO; JPO; DERWENT	OR	OFF	2004/11/19 12:09
L18	72	heptatrieno\$	USPAT; EPO; JPO; DERWENT	OR	OFF	2004/11/19 12:09
L19	1	histone and heptatrieno\$	USPAT; EPO; JPO; DERWENT	OR	OFF	2004/11/19 12:09
L20	556	heptatrien\$	USPAT; EPO; JPO; DERWENT	OR	OFF	2004/11/19 12:09
L21	38	(Histone adj deacetylase) and hydroxamic	USPAT; EPO; JPO; DERWENT	OR	OFF	2004/11/19 12:09
L22	3	"2001038322".pn.	USPAT; EPO; JPO; DERWENT	OR	OFF	2004/11/19 12:09
L23	3	"9814424".pn.	USPAT; EPO; JPO; DERWENT	OR	OFF	2004/11/19 12:09
L24	239	(562/491).CCLS.	USPAT; USOCR; EPO; JPO; DERWENT	OR	OFF	2004/11/19 12:09
L25	48	heptatrienoic	USPAT; EPO; JPO; DERWENT	OR	OFF	2004/11/19 12:09
L26	3	7-phenyl-2,4,6-heptatrieno\$	USPAT; EPO; JPO; DERWENT	OR	OFF	2004/11/19 12:09
L27	2	"5037813".pn.	USPAT; EPO; JPO; DERWENT	OR	OFF	2004/11/19 12:09
L28	322	(562/495).CCLS.	USPAT; USOCR; EPO; JPO; DERWENT	OR	OFF	2004/11/19 12:09

L29	2	"4371516".pn.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2004/11/19 12:09
L30	2	"4371516".pn.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2004/11/19 12:09
L31	15073	dodecen\$	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2004/11/19 12:09
L32	70673	insecticid\$	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2004/11/19 12:09
L33	436	dodecen\$ and insecticid\$	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2004/11/19 12:09
L34	16	"2005271"	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2004/11/19 12:09
L35	2	"5747537".pn.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2004/11/19 12:09
L36	3	"9929640".pn.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2004/11/19 12:09
L37	2	"53101527".pn.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2004/11/19 12:09
L38	2	"9827162".pn.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2004/11/19 12:09
L39	2	"4810299".pn.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2004/11/19 12:09
L40	2	"4621099".pn.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2004/11/19 12:09
L41	1	"4621099".URPN.	USPAT	OR	ON	2004/11/19 12:09

L42	2	"5459149".pn.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2004/11/19 12:09
L43	5	"2849466" .pn.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2004/11/19 12:09

	Type	L #	Hits	Search Text	DBs	Time Stamp	Comments
1	BRS	L1	0	7,7-diphenyl-2,4,6-heptatrienoic	USPAT; EPO; JPO; DERWEN T	2004/11/19 12:09	
2	BRS	L2	0	(Histone adj deacetylase) and (("562/495").CCLS.)	USPAT; EPO; JPO; DERWEN T	2004/11/19 12:09	
3	IS&R	L3	0	("17and117").PN.	USPAT; USOCR; EPO; JPO; DERWEN T	2004/11/19 12:09	
4	BRS	L4	0	heptatrieno\$ and (("562/491").CCLS.)	USPAT; EPO; JPO; DERWEN T	2004/11/19 12:09	
5	BRS	L5	0	heptatrien\$ and (("562/491").CCLS.)	USPAT; EPO; JPO; DERWEN T	2004/11/19 12:09	
6	BRS	L6	0	(dodecen\$ and insecticid\$) and "2005271"	US- PGPUB; USPAT; EPO; JPO; DERWEN T	2004/11/19 12:09	
7	IS&R	L7	279	(514/559).CCLS.	USPAT; USOCR; EPO; JPO; DERWEN T	2004/11/19 12:09	

8	IS&R	L8	885	(514/562) .CCLS.	USPAT; USOCR; EPO; JPO; DERWEN T	2004/11/19 12:09	
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	Error Definition	Errors
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	Type	L #	Hits	Search Text	DBs	Time Stamp	Comments
9	IS&R	L9	414	(514/564) .CCLS.	USPAT; USOCR; EPO; JPO; DERWEN T	2004/11/19 12:09	
10	IS&R	L10	716	(514/570) .CCLS.	USPAT; USOCR; EPO; JPO; DERWEN T	2004/11/19 12:09	
11	IS&R	L11	179	(514/571) .CCLS.	USPAT; USOCR; EPO; JPO; DERWEN T	2004/11/19 12:09	
12	BRS	L16	1	heptatrienoic and histone	USPAT; EPO; JPO; DERWEN T	2004/11/19 12:09	
13	BRS	L17	1	7-phenyl-2,4,6-heptatrienoic	USPAT; EPO; JPO; DERWEN T	2004/11/19 12:09	
14	BRS	L19	1	histone and heptatrieno\$	USPAT; EPO; JPO; DERWEN T	2004/11/19 12:09	
15	BRS	L41	1	"4621099" .URPN.	USPAT	2004/11/19 12:09	
16	BRS	L12	2	"53101527" .pn.	US- PGPUB; USPAT; EPO; JPO; DERWEN T	2004/11/19 12:09	

	Error Definition	Errors
9		
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	Type	L #	Hits	Search Text	DBs	Time Stamp	Comments
17	BRS	L18	72	heptatrieno\$	USPAT; EPO; JPO; DERWEN T	2004/11/19 12:09	
18	BRS	L21	38	(Histone adj deacetylase) and hydroxamic	USPAT; EPO; JPO; DERWEN T	2004/11/19 12:09	
19	BRS	L22	3	"2001038322".pn.	USPAT; EPO; JPO; DERWEN T	2004/11/19 12:09	
20	BRS	L23	3	"9814424".pn.	USPAT; EPO; JPO; DERWEN T	2004/11/19 12:09	
21	BRS	L25	48	heptatrienoic	USPAT; EPO; JPO; DERWEN T	2004/11/19 12:09	
22	BRS	L26	3	7-phenyl-2,4,6- heptatrieno\$	USPAT; EPO; JPO; DERWEN T	2004/11/19 12:09	
23	BRS	L27	2	"5037813".pn.	USPAT; EPO; JPO; DERWEN T	2004/11/19 12:09	
24	BRS	L29	2	"4371516".pn.	US- PGPUB; USPAT; EPO; JPO; DERWEN T	2004/11/19 12:09	

	Error Definition	Errors
17		
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	Type	L #	Hits	Search Text	DBs	Time Stamp	Comments
25	BRS	L30	2	"4371516".pn.	US- PGPUB; USPAT; EPO; JPO; DERWEN T	2004/11/19 12:09	
26	BRS	L34	16	"2005271"	US- PGPUB; USPAT; EPO; JPO; DERWEN T	2004/11/19 12:09	
27	BRS	L35	2	"5747537".pn.	US- PGPUB; USPAT; EPO; JPO; DERWEN T	2004/11/19 12:09	
28	BRS	L36	3	"9929640".pn.	US- PGPUB; USPAT; EPO; JPO; DERWEN T	2004/11/19 12:09	
29	BRS	L37	2	"53101527".pn.	US- PGPUB; USPAT; EPO; JPO; DERWEN T	2004/11/19 12:09	
30	BRS	L38	2	"9827162".pn.	US- PGPUB; USPAT; EPO; JPO; DERWEN T	2004/11/19 12:09	

31	BRS	L39	2	"4810299".pn.	US- PGPUB; USPAT; EPO; JPO; DERWEN T	2004/11/19 12:09	
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	Error Definition	Errors
25		
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31		
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	Type	L #	Hits	Search Text	DBs	Time Stamp	Comments
32	BRS	L40	2	"4621099".pn.	US- PGPUB; USPAT; EPO; JPO; DERWEN T	2004/11/19 12:09	
33	BRS	L42	2	"5459149".pn.	US- PGPUB; USPAT; EPO; JPO; DERWEN T	2004/11/19 12:09	
34	BRS	L43	5	"2849466" .pn.	US- PGPUB; USPAT; EPO; JPO; DERWEN T	2004/11/19 12:09	
35	IS&R	L24	239	(562/491).CCLS.	USPAT; USOCR; EPO; JPO; DERWEN T	2004/11/19 12:09	
36	IS&R	L28	322	(562/495).CCLS.	USPAT; USOCR; EPO; JPO; DERWEN T	2004/11/19 12:09	
37	BRS	L13	456	Histone adj deacetylase	USPAT; EPO; JPO; DERWEN T	2004/11/19 12:09	

38	BRS	L33	436	dodecen\$ and insecticid\$	US- PGPUB; USPAT; EPO; JPO; DERWEN T	2004/11/19 12:09	
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	Error Definition	Errors
32		
33		
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37		

38		
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	Type	L #	Hits	Search Text	DBs	Time Stamp	Comments
39	BRS	L20	556	heptatrien\$	USPAT; EPO; JPO; DERWEN T	2004/11/19 12:09	
40	BRS	L14	5855	hydroxamic	USPAT; EPO; JPO; DERWEN T	2004/11/19 12:09	
41	BRS	L15	3694	histone	USPAT; EPO; JPO; DERWEN T	2004/11/19 12:09	
42	BRS	L31	15073	dodecen\$	US- PGPUB; USPAT; EPO; JPO; DERWEN T	2004/11/19 12:09	
43	BRS	L32	70673	insecticid\$	US- PGPUB; USPAT; EPO; JPO; DERWEN T	2004/11/19 12:09	

	Error Definition	Errors
39		
40		
41		
42		
43		

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

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NEWS 3 JUL 12 BEILSTEIN enhanced with new display and select options,
resulting in a closer connection to BABS
NEWS 4 AUG 02 IFIPAT/IFIUDB/IFICDB reloaded with new search and display
fields
NEWS 5 AUG 02 CAPLUS and CA patent records enhanced with European and Japan
Patent Office Classifications
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NEWS 8 AUG 27 BIOTECHABS/BIOTECHDS: Two new display fields added for legal
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NEWS 15 NOV 18 Current-awareness alerts, saved answer sets, and current
search transcripts to be affected by CERAB, COMPUAB, ELCOM,
and SOLIDSTATE reloads

NEWS EXPRESS OCTOBER 29 CURRENT WINDOWS VERSION IS V7.01A, CURRENT
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
NEWS HOURS STN Operating Hours Plus Help Desk Availability
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NEWS PHONE Direct Dial and Telecommunication Network Access to STN
NEWS WWW CAS World Wide Web Site (general information)

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 06:21:17 ON 19 NOV 2004

=> logoff hold

COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
0.21	0.21

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 06:21:28 ON 19 NOV 2004

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

***** RECONNECTED TO STN INTERNATIONAL *****
SESSION RESUMED IN FILE 'HOME' AT 06:39:58 ON 19 NOV 2004
FILE 'HOME' ENTERED AT 06:39:58 ON 19 NOV 2004

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 06:40:07 ON 19 NOV 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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STRUCTURE FILE UPDATES: 17 NOV 2004 HIGHEST RN 783276-57-3
DICTIONARY FILE UPDATES: 17 NOV 2004 HIGHEST RN 783276-57-3

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

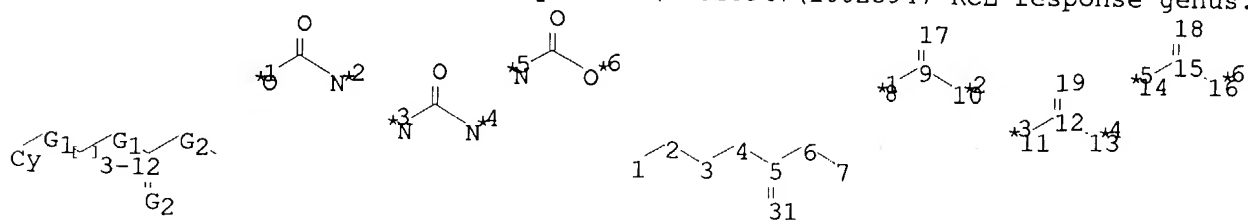
Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\Examination Auxillary files\10025947\10025947 RCE response genus.str



chain nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 31
chain bonds :
1-2 2-3 3-4 4-5 5-6 5-31 6-7 8-9 9-10 9-17 11-12 12-13 12-19 14-15
15-16 15-18
exact/norm bonds :
1-2 2-3 3-4 4-5 5-6 5-31 6-7 8-9 9-10 9-17 11-12 12-13 12-19 14-15
15-16 15-18

G1:O,S,CH2,N,[*1-*2],[*3-*4],[*5-*6]

G2:O,S

Match level :

1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS
31:CLASS

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> search l1 sss sam

SAMPLE SEARCH INITIATED 06:40:59 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 370059 TO ITERATE

0.3% PROCESSED 1000 ITERATIONS

14 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**

PROJECTED ITERATIONS: EXCEEDS 1000000

PROJECTED ANSWERS: EXCEEDS 99301

L2 14 SEA SSS SAM L1

=> d scan

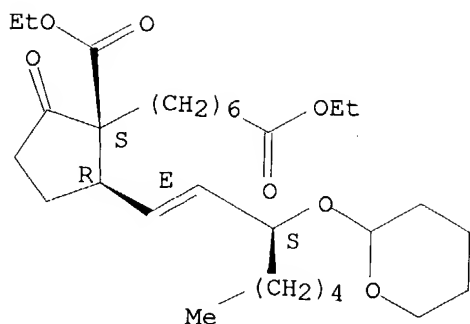
L2 14 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN Prost-13-ene-8-carboxylic acid, 1-ethoxy-1,9-dioxo-15-[(tetrahydro-2H-
pyran-2-yl)oxy]-, ethyl ester, (13E,15S)-(±)-(9CI)

MF C30 H50 O7

Relative stereochemistry.

Double bond geometry as shown.

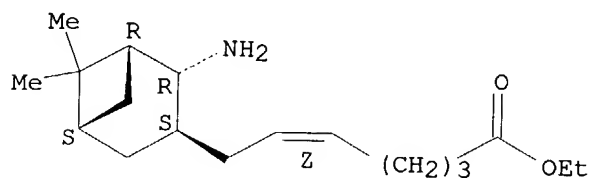


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

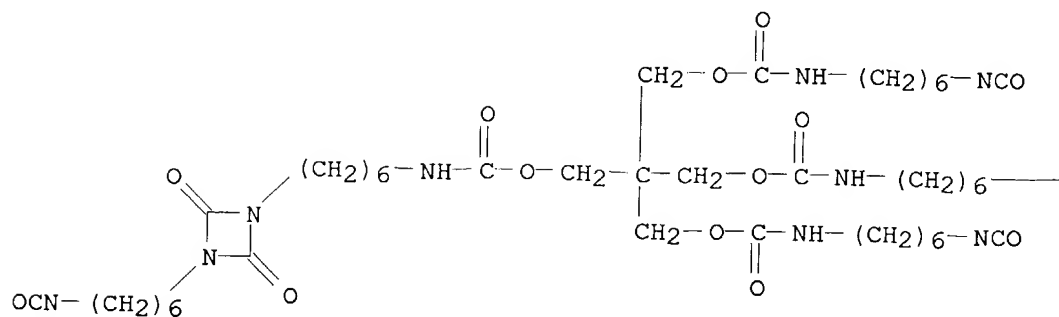
L2 14 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 5-Heptenoic acid, 7-[(1R,2R,3S,5S)-2-amino-6,6-dimethylbicyclo[3.1.1]hept-3-yl]-, ethyl ester, (5Z)- (9CI)
 MF C18 H31 N O2
 CI COM

Absolute stereochemistry. Rotation (+).
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

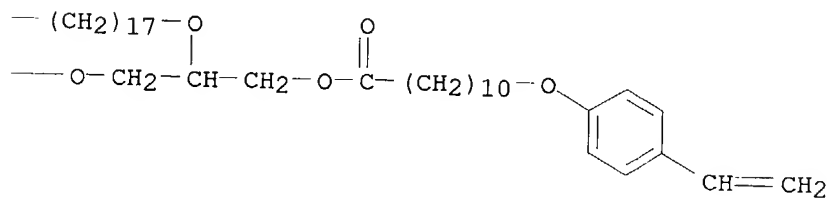
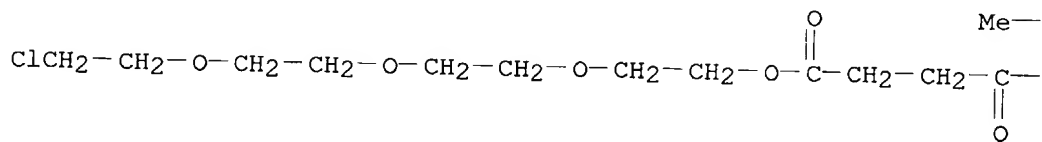
L2 14 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Carbamic acid, (6-isocyanatoethyl)-, 2-[[[[(6-isocyanatoethyl)amino]carbonyl]oxy]methyl]-2-[[[[(6-isocyanatoethyl)-2,4-dioxo-1,3-diazetidin-1-yl]hexyl]amino]carbonyl]oxy]methyl]-1,3-propanediyl ester (9CI)
 MF C45 H72 N10 O14
 CI COM



—NCO

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

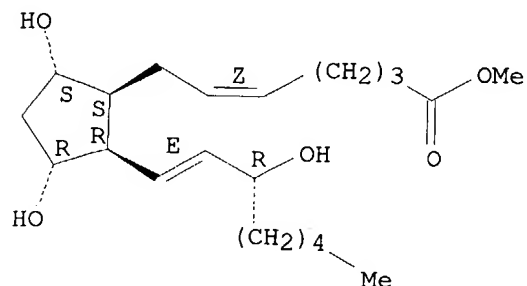
L2 14 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Butanedioic acid, 2-[2-[2-(2-chloroethoxy)ethoxy]ethoxy]ethyl
 3-[[11-(4-ethenylphenoxy)-1-oxoundecyl]oxy]-2-(octadecyloxy)propyl ester
 (9CI)
 MF C52 H89 Cl O11



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 14 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Prosta-5,13-dien-1-oic acid, 9,11,15-trihydroxy-, methyl ester,
 (5Z,8β,9α,11α,13E,15R)- (9CI)
 MF C21 H36 O5

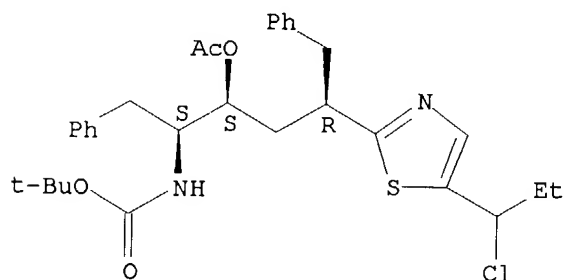
Absolute stereochemistry. Rotation (+).
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 14 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Carbamic acid, [(1S,2S,4R)-2-(acetyloxy)-4-[5-(1-chloropropyl)-2-thiazolyl]-5-phenyl-1-(phenylmethyl)pentyl]-, 1,1-dimethylethyl ester
 (9CI)
 MF C31 H39 Cl N2 O4 S

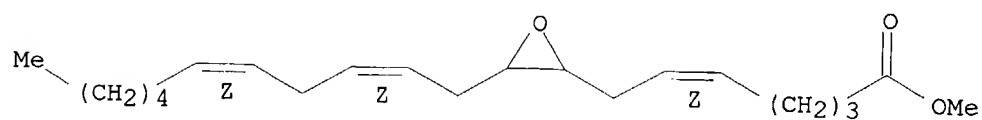
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 14 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 5-Heptenoic acid, 7-[3-(2Z,5Z)-2,5-undecadienyloxiranyl]-, methyl ester,
 (5Z)- (9CI)
 MF C21 H34 O3

Double bond geometry as shown.

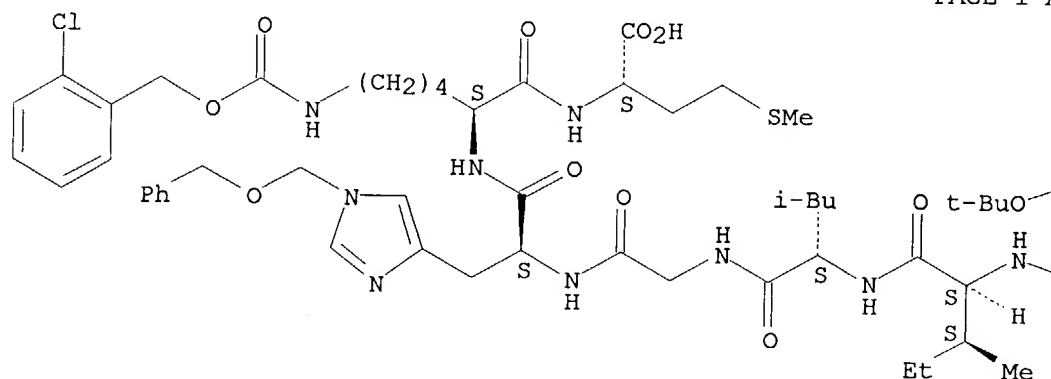


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

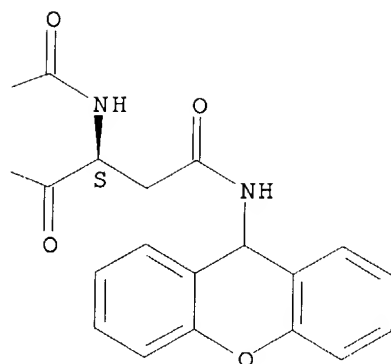
L2 14 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN L-Methionine, N2-[(1,1-dimethylethoxy)carbonyl]-N-9H-xanthen-9-yl-L-
 asparaginyl-L-isoleucyl-L-leucylglycyl-1-[(phenylmethoxy)methyl]-L-
 histidyl-N6-[[(2-chlorophenyl)methoxy]carbonyl]-L-lysyl- (9CI)
 SQL 7
 MF C69 H90 Cl N11 O15 S

Absolute stereochemistry.

PAGE 1-A

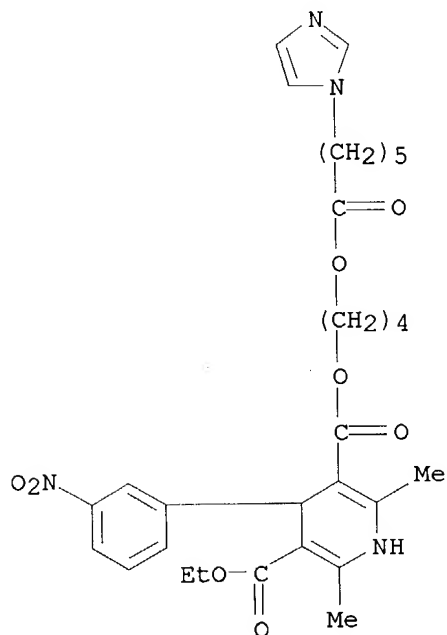


PAGE 1-B



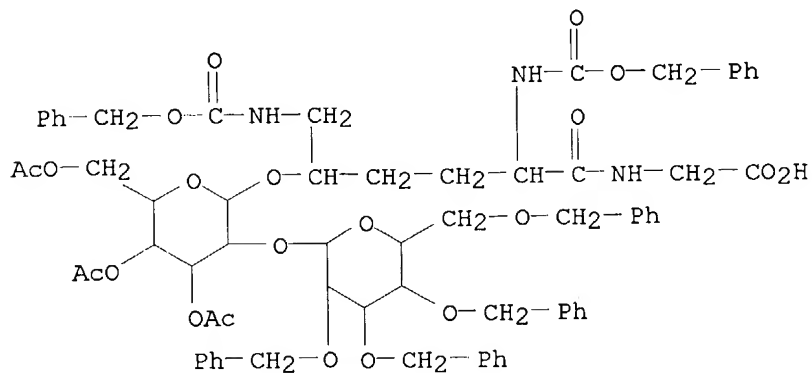
L2 14 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN 3,5-Pyridinedicarboxylic acid, 1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-
 , ethyl 4-[[6-(1H-imidazol-1-yl)-1-oxohexyl]oxy]butyl ester (9CI)
 MF C30 H38 N4 O8



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

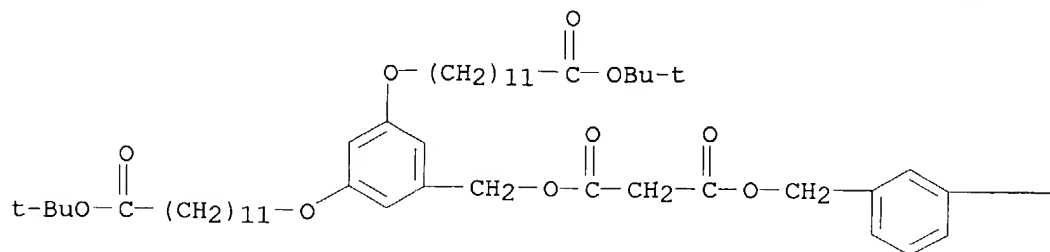
L2 14 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Glycine, N-[N2,N6-bis[(phenylmethoxy)carbonyl]-threo-5-[[3,4,6-tri-O-
 acetyl-2-O-[2,3,4,6-tetrakis-O-(phenylmethyl)-α-D-glucopyranosyl]-
 β-D-galactopyranosyl]oxy]-L-lysyl]- (9CI)
 MF C70 H79 N3 O21



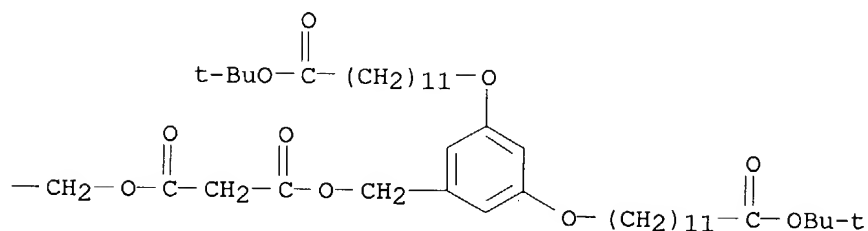
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 14 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Propanedioic acid, 1,3-phenylenebis(methylene) bis[[3,5-bis[[12-(1,1-dimethylethoxy)-12-oxododecyl]oxy]phenyl]methyl] ester (9CI)
 MF C92 H146 O20

PAGE 1-A



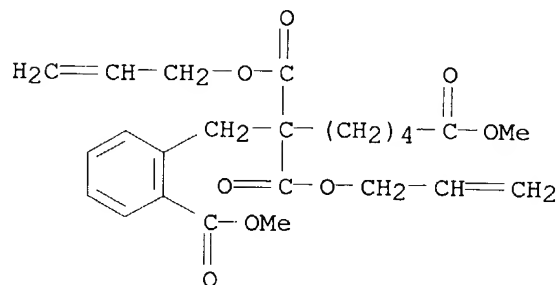
PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

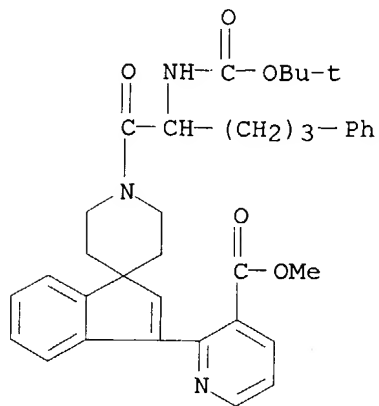
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):4

L2 14 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 1,1,5-Pentanetricarboxylic acid, 1-[[2-(methoxycarbonyl)phenyl]methyl]-, 5-methyl 1,1-di-2-propenyl ester (9CI)
 MF C24 H30 O8



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

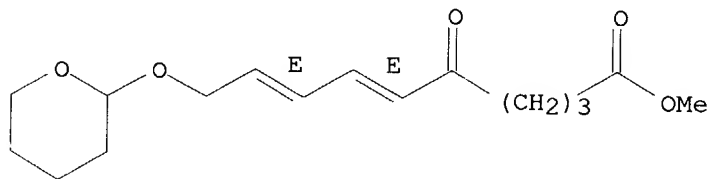
L2 14 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 3-Pyridinecarboxylic acid, 2-[1'-[2-[[(1,1-dimethylethoxy) carbonyl] amino]-
 1-oxo-5-phenylpentyl]spiro[1H-indene-1,4'-piperidin]-3-yl]-, methyl ester
 (9CI)
 MF C36 H41 N3 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 14 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 6,8-Decadienoic acid, 5-oxo-10-[(tetrahydro-2H-pyran-2-yl)oxy]-, methyl
 ester, (E,E)- (9CI)
 MF C16 H24 O5

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> logoff hold

COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
2.10	2.31

SESSION WILL BE HELD FOR 60 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 06:42:50 ON 19 NOV 2004

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

***** RECONNECTED TO STN INTERNATIONAL *****
SESSION RESUMED IN FILE 'REGISTRY' AT 06:46:26 ON 19 NOV 2004
FILE 'REGISTRY' ENTERED AT 06:46:26 ON 19 NOV 2004
COPYRIGHT (C) 2004 American Chemical Society (ACS)

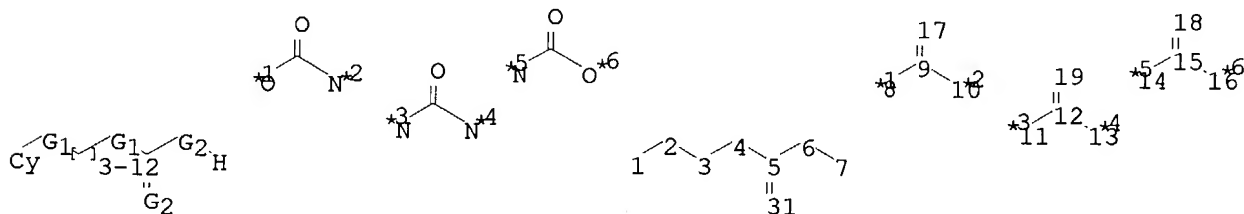
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
2.10	2.31

FULL ESTIMATED COST

=>

Uploading C:\Examination Auxillary files\10025947\10025947 RCE response genus acids.str



chain nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 31

chain bonds :

1-2 2-3 3-4 4-5 5-6 5-31 6-7 8-9 9-10 9-17 11-12 12-13 12-19 14-15
15-16 15-18

exact/norm bonds :

1-2 2-3 3-4 4-5 5-6 5-31 6-7 8-9 9-10 9-17 11-12 12-13 12-19 14-15
15-16 15-18

G1:O,S,CH2,N,[*1-*2],[*3-*4],[*5-*6]

G2:O,S

Match level :

1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS
31:CLASS

L3 STRUCTURE UPLOADED

=> d l3
L3 HAS NO ANSWERS
L3 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> search l3 sss sam
SAMPLE SEARCH INITIATED 06:46:58 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 661419 TO ITERATE

0.2% PROCESSED 1000 ITERATIONS 11 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

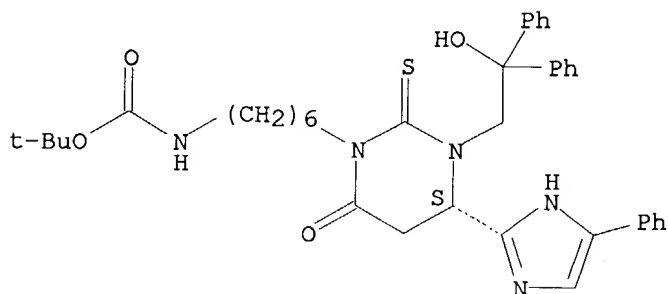
FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: EXCEEDS 1000000
PROJECTED ANSWERS: EXCEEDS 140400

L4 11 SEA SSS SAM L3

=> d scan

L4 11 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Carbamic acid, [6-[(4S)-tetrahydro-3-(2-hydroxy-2,2-diphenylethyl)-6-oxo-4-(4-phenyl-1H-imidazol-2-yl)-2-thioxo-1(2H)-pyrimidinyl]hexyl]-, 1,1-dimethylethyl ester (9CI)
MF C38 H45 N5 O4 S

Absolute stereochemistry.

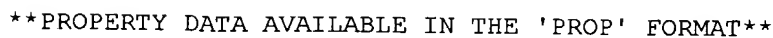


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):11

L4 11 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Carbamic acid, [(1S,2S,4R)-2-(acetyloxy)-4-[5-(1-chloropropyl)-2-thiazolyl]-5-phenyl-1-(phenylmethyl)pentyl]-, 1,1-dimethylethyl ester (9CI)
MF C31 H39 Cl N2 O4 S

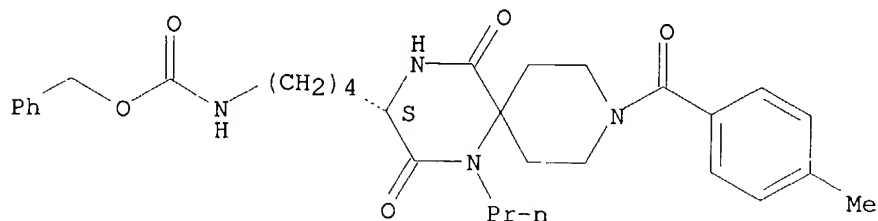
Absolute stereochemistry.



Absolute stereochemistry.
Double bond geometry as shown.



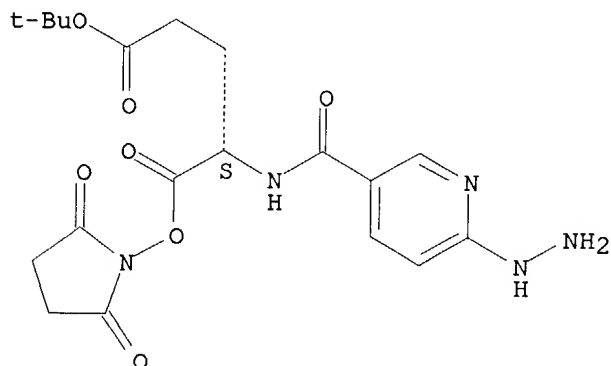
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 11 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Pentanoic acid, 5-[(2,5-dioxo-1-pyrrolidinyl)oxy]-4-[[6-hydrazino-3-pyridinyl)carbonyl]amino]-5-oxo-, 1,1-dimethylethyl ester, (4S)- (9CI)
MF C19 H25 N5 O7
CI COM

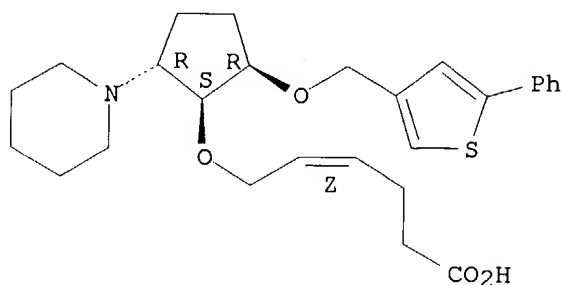
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

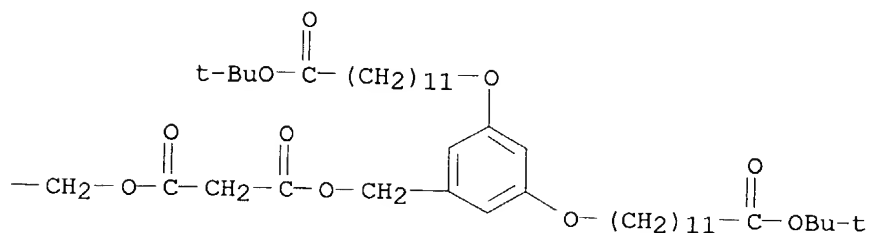
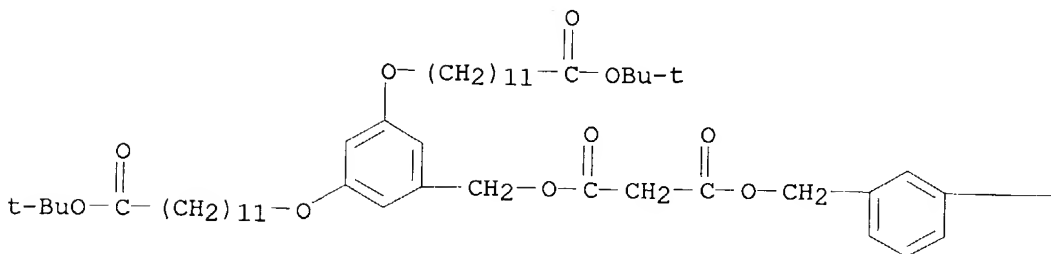
L4 11 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 4-Hexenoic acid, 6-[[2-[(5-phenyl-3-thienyl)methoxy]-5-(1-piperidinyl)cyclopentyl]oxy]-, [1 α (Z),2 α ,5 β]- (9CI)
MF C27 H35 N O4 S

Relative stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

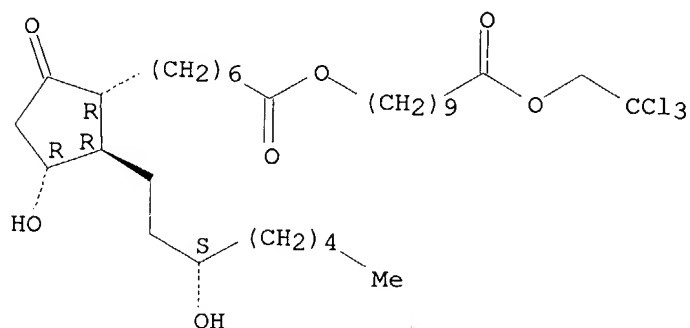
L4 11 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Propanedioic acid, 1,3-phenylenebis(methylene) bis[[3,5-bis[[12-(1,1-dimethylethoxy)-12-oxododecyl]oxy]phenyl]methyl] ester (9CI)
MF C92 H146 O20



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 11 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Prostan-1-oic acid, 11,15-dihydroxy-9-oxo-, 10-oxo-10-(2,2,2-trichloroethoxy)decyl ester, (11 α ,15S)- (9CI)
 MF C32 H55 Cl3 O7

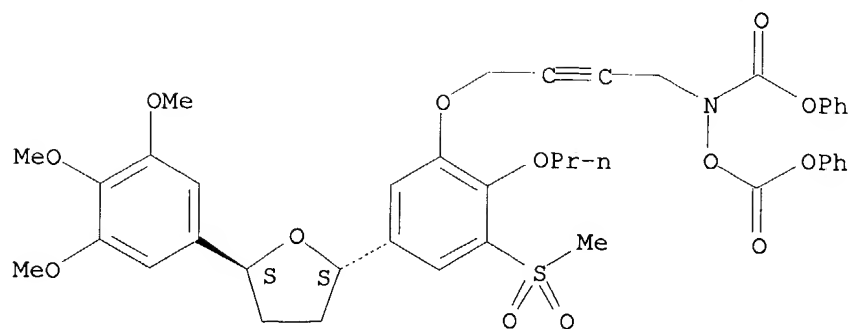
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

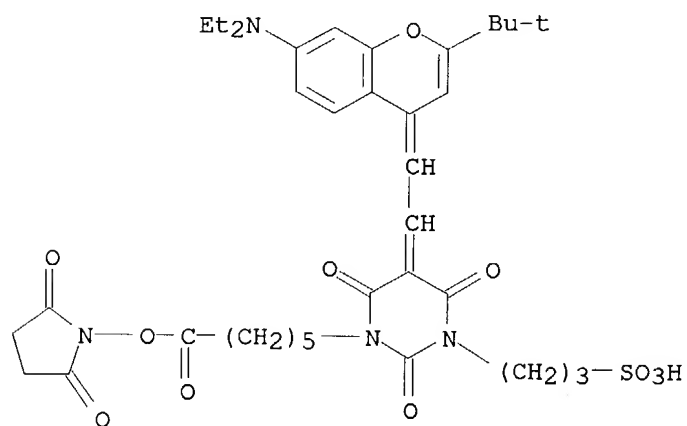
L4 11 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Carbamic acid, [4-[3-(methylsulfonyl)-2-propoxy-5-[tetrahydro-5-(3,4,5-trimethoxyphenyl)-2-furanyl]phenoxy]-2-butynyl][(phenoxycarbonyl)oxy]-, phenyl ester, trans- (9CI)
 MF C41 H43 N O13 S

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

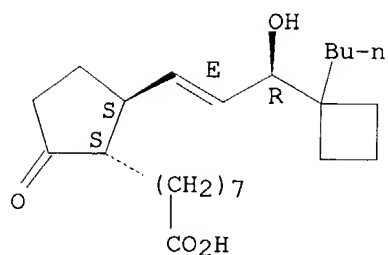
L4 11 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 1(2H)-Pyrimidinepropanesulfonic acid, 5-[[7-(diethylamino)-2-(1,1-dimethylethyl)-4H-1-benzopyran-4-ylidene]ethylidene]-3-[6-[(2,5-dioxo-1-pyrrolidinyl)oxy]-6-oxohexyl]tetrahydro-2,4,6-trioxo-, sodium salt (9CI)
 MF C36 H46 N4 O11 S . Na



● Na

L4 11 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Cyclopentaneoctanoic acid, 2-[3-(1-butylcyclobutyl)-3-hydroxy-1-propenyl]-5-oxo-, [1 α ,2 β (1E,3S*)]- (9CI)
 MF C24 H40 O4

Relative stereochemistry.
 Double bond geometry as shown.

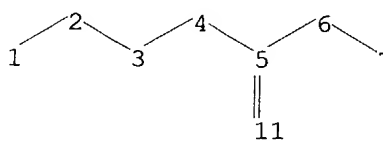
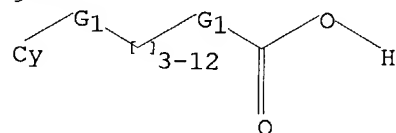


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=>

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genus.str



chain nodes :

1 2 3 4 5 6 7 11

chain bonds :

1-2 2-3 3-4 4-5 5-6 5-11 6-7

exact/norm bonds :

1-2 2-3 3-4 4-5

exact bonds :

6-7

normalized bonds :

5-6 5-11

G1:O,S,N,CH2

Match level :

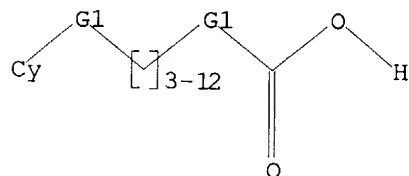
1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 11:CLASS

L5 STRUCTURE UPLOADED

=> d 15

L5 HAS NO ANSWERS

L5 STR



G1 O,S,N,CH2

Structure attributes must be viewed using STN Express query preparation.

=> search 15 sss sam

SAMPLE SEARCH INITIATED 06:51:50 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 113352 TO ITERATE

0.9% PROCESSED 1000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

21 ANSWERS

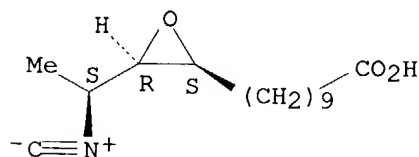
FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: EXCEEDS 1000000
PROJECTED ANSWERS: EXCEEDS 44681

L6 21 SEA SSS SAM L5

=> d scan

L6 21 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Oxiranedecanoic acid, 3-(1-isocyanoethyl)-, [2 α ,3 α (R*)]- (9CI)
MF C15 H25 N O3

Relative stereochemistry.



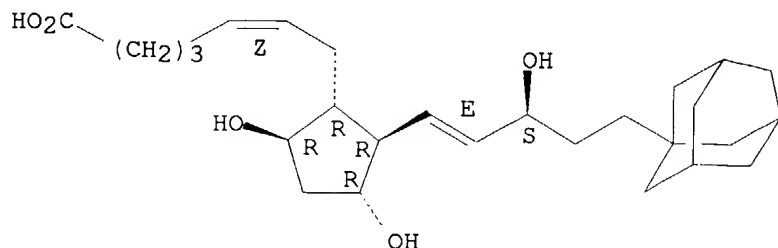
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):21

L6 21 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 5-Heptenoic acid, 7-[3,5-dihydroxy-2-(3-hydroxy-5-tricyclo[3.3.1.1^{3,7}]dec-1-yl-1-pentenyl)cyclopentyl]-, [1R-[1 α (Z),2 β (1E,3S*),3 α ,5 β]]-, compd. with 2-amino-2-(hydroxymethyl)-1,3-propanediol (1:1)
(9CI)

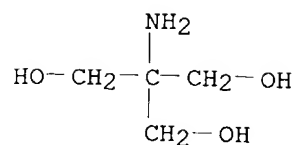
MF C27 H42 O5 . C4 H11 N O3

CM 1

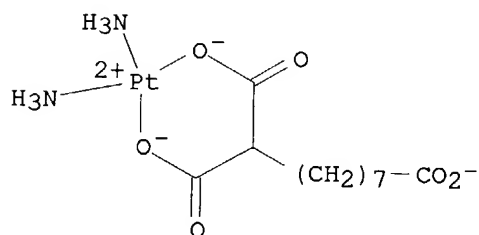
Absolute stereochemistry.
Double bond geometry as shown.



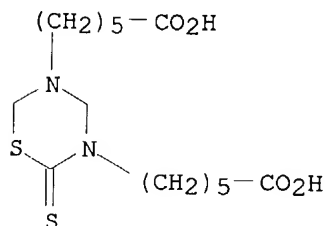
CM 2



L6 21 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Platinate(1-), diammine[1,1,8-octanetricarboxylato(3-)]-, hydrogen,
(SP-4-2)- (9CI)
MF C11 H21 N2 O6 Pt . H
CI CCS



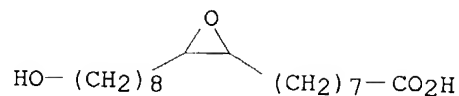
L6 21 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2H-1,3,5-Thiadiazine-3,5(4H,6H)-dihexanoic acid, 2-thioxo- (8CI, 9CI)
MF C15 H26 N2 O4 S2



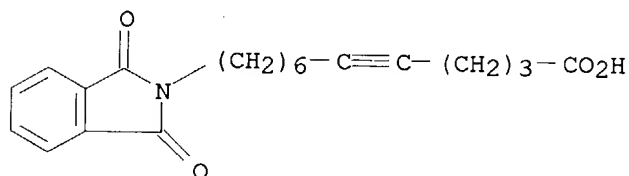
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 21 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Oxiraneoctanoic acid, 3-(8-hydroxyoctyl)-, didehydro deriv. (9CI)

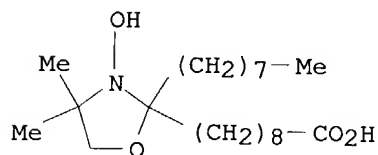
MF C18 H32 O4
 CI IDS
 CM 1



L6 21 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 5-Dodecynoic acid, 12-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)- (9CI)
 MF C20 H23 N O4



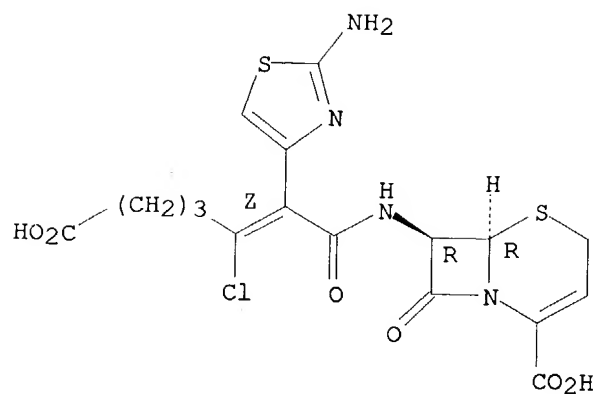
L6 21 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2-Oxazolidinenonanoic acid, 3-hydroxy-4,4-dimethyl-2-octyl-, monopotassium salt (9CI)
 MF C22 H43 N O4 . K



● K

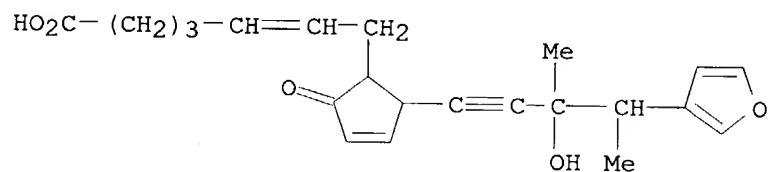
L6 21 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 7-[[2-(2-amino-4-thiazolyl)-6-carboxy-3-chloro-1-oxo-2-hexenyl]amino]-8-oxo-, [6R-[6α,7β(Z)]]- (9CI)
 MF C17 H17 Cl N4 O6 S2
 CI COM

Absolute stereochemistry.
 Double bond geometry as shown.



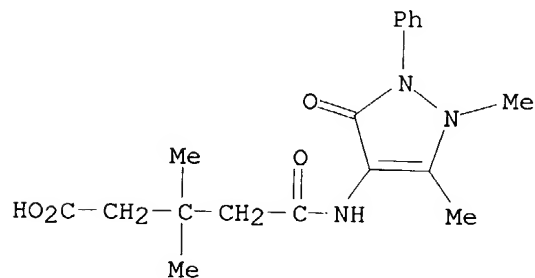
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 21 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 5-Heptenoic acid, 7-[2-[4-(3-furanyl)-3-hydroxy-3-methyl-1-pentynyl]-5-oxo-
 3-cyclopenten-1-yl]- (9CI)
 MF C22 H26 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

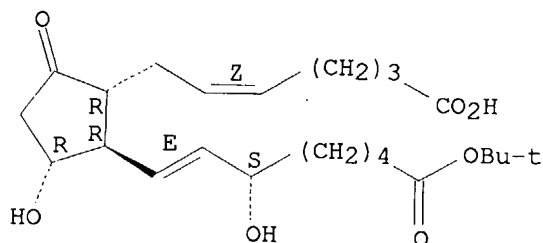
L6 21 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Pentanoic acid, 5-[(2,3-dihydro-1,5-dimethyl-3-oxo-2-phenyl-1H-pyrazol-4-
 yl)amino]-3,3-dimethyl-5-oxo- (9CI)
 MF C18 H23 N3 O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

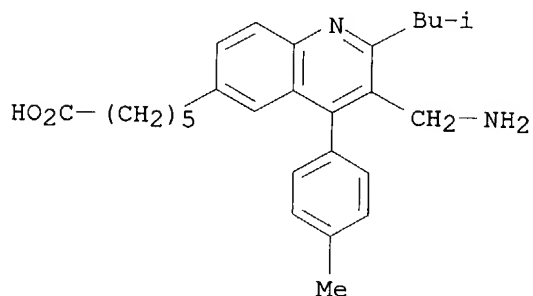
L6 21 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Prosta-5,13-diene-1,20-dioic acid, 11,15-dihydroxy-9-oxo-,
20-(1,1-dimethylethyl) ester, (5Z,11 α ,13E,15S)- (9CI)
MF C24 H38 O7

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

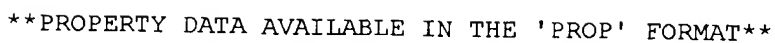
L6 21 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 6-Quinolinehexanoic acid, 3-(aminomethyl)-4-(4-methylphenyl)-2-(2-methylpropyl)-, dihydrochloride (9CI)
MF C27 H34 N2 O2 . 2 Cl H



● 2 HCl

L6 21 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 4-Imidazolidineheptanoic acid, 3-(3-cyclopentyl-3-hydroxypropyl)-2,5-dioxo-, (R*,S*)- (9CI)
MF C18 H30 N2 O5

Relative stereochemistry.

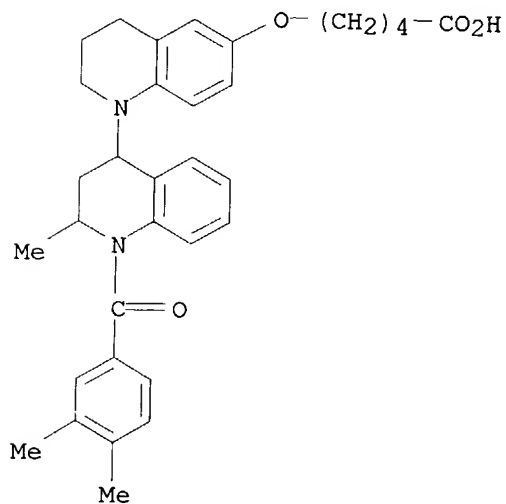


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

$$\begin{array}{c} \text{O} \\ \parallel \\ \text{C}_6\text{H}_{10} \end{array} \begin{array}{l} \text{CH}_2\text{---CH}_2\text{---CH(OH)---(CH}_2\text{)}_4\text{---Me} \\ \text{CH}_2\text{---CH}_2\text{---CH=CH---CH}_2\text{---CH}_2\text{---CO}_2\text{H} \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

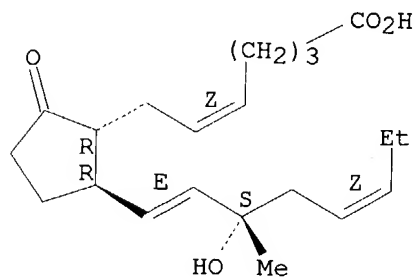
L6 21 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Pentanoic acid, 5-[[1'-(3,4-dimethylbenzoyl)-1',2',3,3',4,4'-hexahydro-2'-methyl[1(2H),4'-biquinolin]-6-yl]oxy]- (9CI)
MF C33 H38 N2 O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 21 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Prosta-5,13,17-trien-1-oic acid, 15-hydroxy-15-methyl-9-oxo-, (5Z,13E,15S,17Z)- (9CI)
MF C21 H32 O4

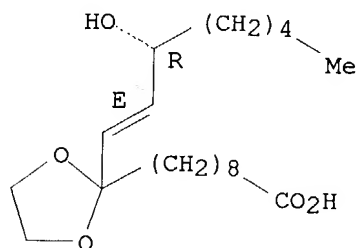
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 21 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 1,3-Dioxolane-2-nonanoic acid, 2-[(1E,3R)-3-hydroxy-1-octenyl]- (9CI)
 MF C20 H36 O5

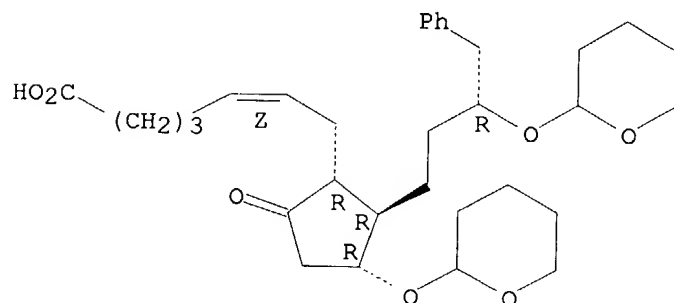
Absolute stereochemistry. Rotation (-).
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

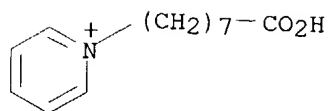
L6 21 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 5-Heptenoic acid, 7-[5-oxo-2-[4-phenyl-3-[(tetrahydro-2H-pyran-2-yl)oxy]butyl]-3-[(tetrahydro-2H-pyran-2-yl)oxy]cyclopentyl]-, [1R-[1 α (Z),2 β (R*),3 α]]- (9CI)
 MF C32 H46 O7

Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 21 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Pyridinium, 1-(7-carboxyheptyl)-, hydroxide, monohydrate (9CI)
 MF C13 H20 N O2 . H2 O . H O

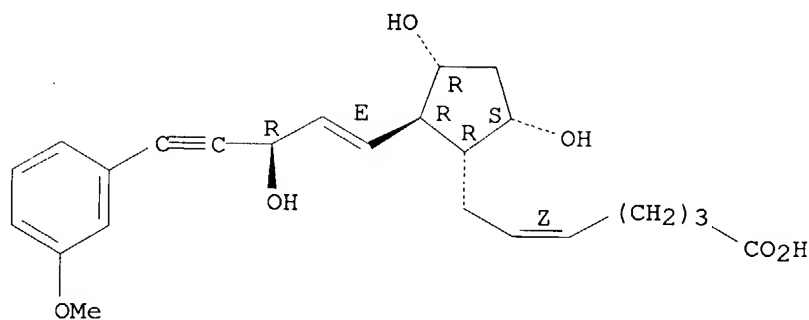


● OH⁻

● H₂O

L6 21 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 5-Heptenoic acid, 7-[3,5-dihydroxy-2-[3-hydroxy-5-(3-methoxyphenyl)-1-penten-4-ynyl]cyclopentyl]-, [1R-[1α(Z),2β(1E,3R*),3α,5.a
 lpha.]]- (9CI)
 MF C24 H30 O6

Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> e Pyridinium, 1-(7-carboxyheptyl)-, hydroxide, monohydrate/cn
 E1 1 PYRIDINIUM, 1-(7-CARBOXYHEPTYL)-, BROMIDE/CN
 E2 1 PYRIDINIUM, 1-(7-CARBOXYHEPTYL)-, CHLORIDE/CN
 E3 1 --> PYRIDINIUM, 1-(7-CARBOXYHEPTYL)-, HYDROXIDE, MONOHYDRATE/CN
 E4 1 PYRIDINIUM, 1-(7-CARBOXYHEPTYL)-, INNER SALT/CN
 E5 1 PYRIDINIUM, 1-(7-CARBOXYHEPTYL)-3-(1-METHYL-2-PYRROLIDINYL)-
 , INNER SALT, (S)-/CN
 E6 1 PYRIDINIUM, 1-(7-CARBOXYHEPTYL)-4-(2-(4-(DIMETHYLAMINO) PHENYL)
 L)ETHENYL)-/CN
 E7 1 PYRIDINIUM, 1-(7-CARBOXYHEPTYL)-4-(2-(4-(DIMETHYLAMINO) PHENYL)
 L)ETHENYL)-, BROMIDE/CN
 E8 1 PYRIDINIUM, 1-(7-CHLORO-2,3-DIHYDRO-1-METHYL-2-OXO-5-PHENYL-

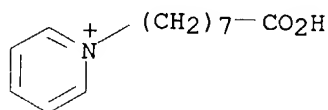
E9 1 1H-1,4-BENZODIAZEPIN-3-YL)-/CN
 PYRIDINIUM, 1-(7-CHLORO-2,3-DIHYDRO-1-METHYL-2-OXO-5-PHENYL-
 1H-1,4-BENZODIAZEPIN-3-YL)-, CHLORIDE/CN
 E10 1 PYRIDINIUM, 1-(7-CHLORO-2,3-DIHYDRO-1-METHYL-2-OXO-5-PHENYL-
 1H-1,4-BENZODIAZEPIN-3-YL)-3-((DIETHYLAMINO) CARBONYL)-/CN
 E11 1 PYRIDINIUM, 1-(7-CHLORO-2,3-DIHYDRO-1-METHYL-2-OXO-5-PHENYL-
 1H-1,4-BENZODIAZEPIN-3-YL)-3-((DIETHYLAMINO) CARBONYL)-, CHLO
 RIDE/CN
 E12 1 PYRIDINIUM, 1-(7-CHLORO-2,3-DIHYDRO-2-OXO-5-PHENYL-1H-1,4-BE
 NZODIAZEPIN-3-YL)-/CN

=> e3

L7 1 "PYRIDINIUM, 1-(7-CARBOXYHEPTYL)-, HYDROXIDE, MONOHYDRATE"/CN

=> d 17

L7 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
 RN 205450-82-4 REGISTRY
 CN **Pyridinium, 1-(7-carboxyheptyl)-, hydroxide, monohydrate (9CI)**
 (CA INDEX NAME)
 MF C13 H20 N O2 . H2 O . H O
 SR CA
 LC STN Files: CA, CAPLUS
 DT.CA Caplus document type: Journal
 RL.NP Roles from non-patents: PREP (Preparation); PRP (Properties)
 CRN (710276-29-2)



● OH⁻

● H₂O

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
16.28	16.49

FULL ESTIMATED COST

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FILE COVERS 1907 - 19 Nov 2004 VOL 141 ISS 21
FILE LAST UPDATED: 17 Nov 2004 (20041117/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> 17

L8 1 L7

=> d 18 ti fbib abs

L8 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN
TI Electrostatic Interactions and Conformations of Zwitterionic Pyridinium Alkanoates
AN 1998:269209 CAPLUS
DN 128:270217
TI Electrostatic Interactions and Conformations of Zwitterionic Pyridinium Alkanoates
AU Szafran, Mirosław; Dega-Szafran, Zofia; Katrusiak, Andrzej; Buczak, Grzegorz; Glowiak, Tadeusz; Sitkowski, Jerzy; Stefaniak, Lech
CS Faculty of Chemistry, A. Mickiewicz University, Poznań, 60-780, Pol.
SO Journal of Organic Chemistry (1998), 63(9), 2898-2908
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
AB Abstract: Conformations of flexible zwitterionic ω -pyridinium alkanoates (PBn) with n methylene units in the tether and their hydrates and hydrochlorides are studied in the solid state by X-ray diffraction, in aqueous solution by FT-IR and ^1H , ^{13}C , and ^{14}N NMR spectroscopies, and in the gas phase by PM3, SAM1, and DFT calcns. PB1 and PB1·H₂O in crystals have a conformation with the N⁺...O intramol. distance of ca. 2.7 Å, while PB3·2H₂O and PB10·3H₂O have a trans-zigzag conformation and are arranged antiparallel. Structures of isolated mols. of ω -pyridinium alkanoates (PBn) and their dihydrates (PBn·2H₂O) and hydrochlorides (PBn·HCl) optimized using the PM3, SAM1, and DFT methods are significantly different from those observed in the crystals. In crystals, when n ≥ 2, as a result of electrostatic interactions in the crystal lattice, the pos. charged center (N⁺ atom) interacts with neg. carboxyl groups, water mols., or chloride ions of the neighboring mols. (intermol. charge compensation), while in the gas phase only with their own (intramol. charge compensation). In aqueous solns., similarly as in the crystalline state, distances between the charged centers increase monotonically with increasing number of methylene units in the tether. The ^1H and ^{13}C NMR data suggest that polymethylene chains in PBn contain more folded (gauche) conformations than do sodium salts of carboxylic acids without a charged N⁺ atom. The SCRF calcns. predict slightly longer N⁺...C_c distances than those derived by Chevalier and Percec for trimethylammonium carboxylates from ^{13}C NMR spectra. This suggests that the SCRF model underestimates contribution of the gauche conformers in aqueous solns.

RE.CNT 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD

ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	5.19	21.68
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-0.70	-0.70

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STRUCTURE FILE UPDATES: 17 NOV 2004 HIGHEST RN 783276-57-3
 DICTIONARY FILE UPDATES: 17 NOV 2004 HIGHEST RN 783276-57-3

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

```
=> e Oxiraneoctanoic acid, 3-(8-hydroxyoctyl)-, didehydro deriv/cn
E1      1      OXIRANEOCTANOIC ACID, 3-(8-HYDROXYOCTYL)-, (2R-CIS)-/CN
E2      1      OXIRANEOCTANOIC ACID, 3-(8-HYDROXYOCTYL)-, CIS-/CN
E3      0 --> OXIRANEOCTANOIC ACID, 3-(8-HYDROXYOCTYL)-, DIDEHYDRO DERIV/C
           N
E4      1      OXIRANEOCTANOIC ACID, 3-(8-HYDROXYOCTYL)-, DIDEHYDRO DERIV./
           CN
E5      1      OXIRANEOCTANOIC ACID, 3-(8-HYDROXYOCTYL)-, METHYL ESTER/CN
E6      1      OXIRANEOCTANOIC ACID, 3-(8-HYDROXYOCTYL)-, METHYL ESTER, CIS
           -/CN
E7      1      OXIRANEOCTANOIC ACID, 3-(8-HYDROXYOCTYL)-, METHYL ESTER, TRA
           NS-/CN
E8      1      OXIRANEOCTANOIC ACID, 3-(8-HYDROXYOCTYL)-, TRANS-(+)-/CN
E9      1      OXIRANEOCTANOIC ACID, 3-(8-HYDROXYOCTYL)-, TRANS-(-)-/CN
E10     1      OXIRANEOCTANOIC ACID, 3-(8-METHOXYOCTYL)-, (2R,3S)-REL-/CN
E11     1      OXIRANEOCTANOIC ACID, 3-(8-OXOOCTYL)-/CN
E12     1      OXIRANEOCTANOIC ACID, 3-(ACETYLOXY)-, METHYL ESTER, CIS-/CN
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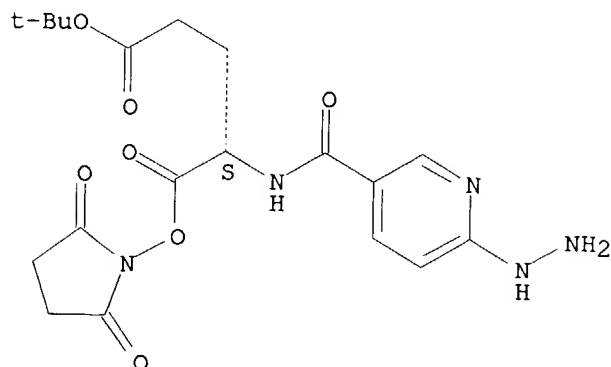
```
=> e4
L9      1 "OXIRANEOCTANOIC ACID, 3-(8-HYDROXYOCTYL)-, DIDEHYDRO DERIV."/CN
```

```
=> d 14
```

```
L4      ANSWER 1 OF 11  REGISTRY  COPYRIGHT 2004 ACS on STN
RN      691844-89-0  REGISTRY
CN      Pentanoic acid, 5-[(2,5-dioxo-1-pyrrolidinyl)oxy]-4-[[6-hydrazino-3-
        pyridinyl)carbonyl]amino]-5-oxo-, 1,1-dimethylethyl ester, (4S)- (9CI)
```

(CA INDEX NAME)
 FS STEREOSEARCH
 MF C19 H25 N5 O7
 CI COM
 SR CA

Absolute stereochemistry.



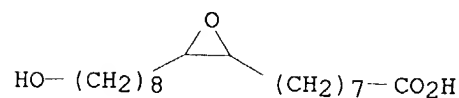
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

=> d 19

L9 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
 RN 75901-10-9 REGISTRY
 CN **Oxiraneoctanoic acid, 3-(8-hydroxyoctyl)-, didehydro deriv. (9CI)**
 (CA INDEX NAME)
 MF C18 H32 O4
 CI IDS
 LC STN Files: CA, CAPLUS
 DT.CA Caplus document type: Journal
 RL.NP Roles from non-patents: BIOL (Biological study)

CM 1

CRN 3233-92-9
 CMF C18 H34 O4



2 REFERENCES IN FILE CA (1907 TO DATE)
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus

COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
8.39	30.07

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
CA SUBSCRIBER PRICE	ENTRY	SESSION
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FILE COVERS 1907 - 19 Nov 2004 VOL 141 ISS 21
 FILE LAST UPDATED: 17 Nov 2004 (20041117/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> 19

L10 2 L9

=> d l10 1-2 ti fbib abs

L10 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
 TI Lipid polymers accumulate in the epidermis and mestome sheath cell walls during low temperature development of winter rye leaves
 AN 1985:403819 CAPLUS
 DN 103:3819
 TI Lipid polymers accumulate in the epidermis and mestome sheath cell walls during low temperature development of winter rye leaves
 AU Griffith, Marilyn; Huner, N. P. A.; Espelie, K. E.; Kolattukudy, P. E.
 CS Dep. Plant Sci., Univ. West. Ontario, London, ON, N6A 5B7, Can.
 SO Protoplasma (1985), 125(1-2), 53-64
 CODEN: PROTA5; ISSN: 0033-183X
 DT Journal
 LA English
 AB Winter rye (*Secale cereale*, cv Puma) was grown at 20° and at 5° and the development of epidermal and mestome sheath cells of leaves from plants grown at both temps. was compared by electron microscopy. At 5° the cells became densely packed with cytoplasm and small vacuoles after 41 days of growth. By day 56 at 5°, epidermal and mestome sheath cells were small in diameter and multivacuolate with asym. thickened walls. By day 76 at 5°, a new developmental stage had been reached in epidermal and mestome sheath cells. The cells were larger in diameter although the thickened cell walls and multivacuolate cytoplasm were still present. As epidermal and mestome sheath cell walls thickened during low temperature growth of winter rye, an increase in cuticle thickness and the deposition of a lamellar layer could be observed in epidermal and mestome sheath cells, resp. The lipid-derived polymers from the leaves of rye plants grown at 20° were shown by reductive depolymn. and gas chromatog.-mass spectroscopy (GC-MS) to be comprised of 18-hydroxy-9,10-epoxyoctadecanoic acid (47%) and dihydroxyhexadecanoic acid (29%). The leaves of plants grown at 5° had 2-4 times as much

lipid-derived polymeric material as those grown at 20° and the proportion of the major monomer, 18-hydroxy-9,10-epoxyoctadecanoic acid, increased to 73% of the polymeric material. Phys. isolation of both epidermal tissue and vascular bundles followed by GC-MS anal. of the monomeric components released by reduction of the resp. lipid polymers showed that 18-hydroxy-9,10-epoxyoctadecanoic acid was the major monomer in the polymer of both the epidermis and the mestome sheaths. The presence of this epoxide monomer in both the cuticle and mestome sheath cell walls of rye leaves was confirmed and visualized by using an epoxide-specific staining reaction.

L10 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
 TI Composition, ultrastructure and function of the cutin- and
 suberin-containing layers in the leaf, fruit peel, juice-sac and inner
 seed coat of grapefruit (Citrus paradisi Macfed.)

AN 1981:12771 CAPLUS

DN 94:12771

TI Composition, ultrastructure and function of the cutin- and
 suberin-containing layers in the leaf, fruit peel, juice-sac and inner
 seed coat of grapefruit (Citrus paradisi Macfed.)

AU Espelie, Karl E.; Davis, Ronald W.; Kolattukudy, P. E.

CS Inst. Biol. Chem., Washington State Univ., Pullman, WA, 99164, USA

SO Planta (1980), 149(5), 498-511

CODEN: PLANAB; ISSN: 0032-0935

DT Journal

LA English

AB Cutin and suberin polymers from various anatomical regions of grapefruit were analyzed chemical and ultrastructurally. The leaf, fruit peel, and juice-sac showed an amorphous cuticular layer. The cutin in the leaf was composed of 10,16-dihydroxy C16 acid and its positional isomers as the major monomers, whereas 16-hydroxy-10-oxo C16 acid was a major component in the fruit peel. Juice-sac cutin, on the other hand, contained the dihydroxy C16 acids, hydroxyoxo C16 acids, hydroxyepoxy C18 acids, and trihydroxy C18 acids. Ultrastructural examination of the inner seed coat showed that an amorphous cuticular layer encircled the entire seed except in the chalazal region which showed several layers of cells with lamellar suberin structure throughout the cell walls. Consistent with the ultrastructural assignment, the compns. of the aliphatic components of the polymers from the chalazal region and the nonchalazal region indicated the presence of suberin and cutin, resp. The aliphatic portion of the polymer from the chalazal region of the inner seed coat contained C16, C18:1, C22, and C24 ω-hydroxy acids (46% combined total) and the corresponding dicarboxylic acids (43%) as the major components. ω-Hydroxy-9,10-epoxy C18 acids and 9,10,18-trihydroxy C18 acids were the major components (77%) of the polymer from the nonchalazal portion of the inner seed coat. The main portion and the chalazal region of the inner seed coat yielded 17 and 342 μg/cm² of aliphatic monomers, resp., and the diffusion resistance of these 2 portions of the inner seed coat were 62 and 192 s/cm, resp. The inner seed coat was the major moisture diffusion barrier influencing imbibition and germination.

=> logoff hold

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
7.30	37.37

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-1.40	-2.10

CA SUBSCRIBER PRICE

SESSION WILL BE HELD FOR 60 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 07:05:11 ON 19 NOV 2004

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Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
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COST IN U.S. DOLLARS	SINCE FILE	TOTAL
FULL ESTIMATED COST	ENTRY	SESSION
	7.30	37.37

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
CA SUBSCRIBER PRICE	ENTRY	SESSION
	-1.40	-2.10

=> file reg

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
FULL ESTIMATED COST	ENTRY	SESSION
	7.74	37.81

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
CA SUBSCRIBER PRICE	ENTRY	SESSION
	-1.40	-2.10

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STRUCTURE FILE UPDATES: 17 NOV 2004 HIGHEST RN 783276-57-3
DICTIONARY FILE UPDATES: 17 NOV 2004 HIGHEST RN 783276-57-3

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

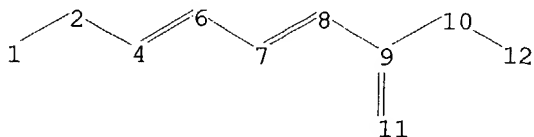
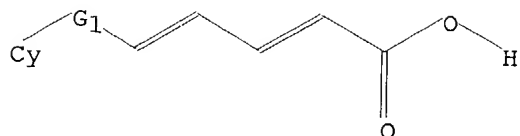
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conducting SmartSELECT searches.

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Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\Examination Auxillary files\10025947\10025947 RCE response 1 st
stab.str



chain nodes :
 1 2 4 6 7 8 9 10 11 12
 chain bonds :
 1-2 2-4 4-6 6-7 7-8 8-9 9-10 9-11 10-12
 exact/norm bonds :
 1-2 2-4
 exact bonds :
 4-6 6-7 7-8 8-9 10-12
 normalized bonds :
 9-10 9-11

G1:O,S,N,CH2

Match level :

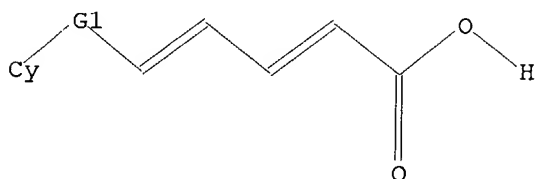
1:Atom 2:CLASS 4:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS
 12:CLASS

L11 STRUCTURE UPLOADED

=> d l11

L11 HAS NO ANSWERS

L11 STR



G1 O,S,N,CH2

Structure attributes must be viewed using STN Express query preparation.

=> search l11 sss

ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:sam

SAMPLE SEARCH INITIATED 07:15:08 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 466 TO ITERATE

100.0% PROCESSED 466 ITERATIONS

SEARCH TIME: 00.00.01

9 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 8025 TO 10615

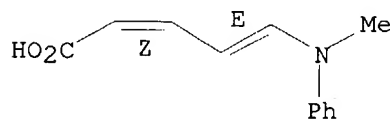
PROJECTED ANSWERS: 9 TO 360

L12 9 SEA SSS SAM L11

=> d scan

L12 9 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2,4-Pentadienoic acid, 5-(methylphenylamino)-, (E,Z)- (9CI)
MF C12 H13 N O2

Double bond geometry as shown.

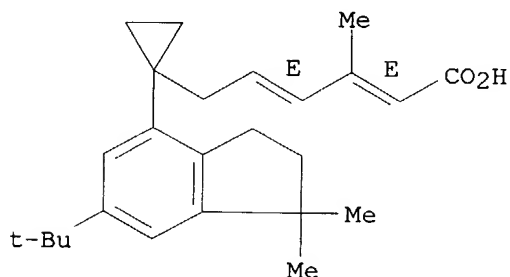


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):9

L12 9 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2,4-Hexadienoic acid, 6-[1-[6-(1,1-dimethylethyl)-2,3-dihydro-1,1-dimethyl-1H-inden-4-yl]cyclopropyl]-3-methyl-, (2E,4E)- (9CI)
MF C25 H34 O2

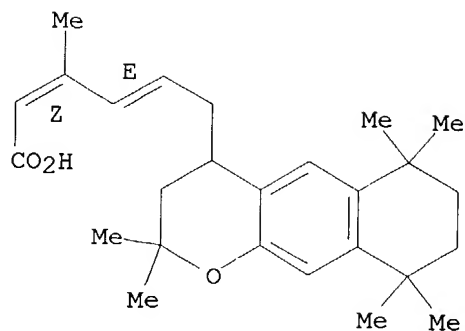
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

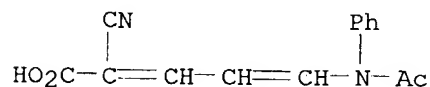
L12 9 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2,4-Hexadienoic acid, 6-(3,4,6,7,8,9-hexahydro-2,2,6,6,9,9-hexamethyl-2H-naphtho[2,3-b]pyran-4-yl)-3-methyl-, (2Z,4E)- (9CI)
MF C26 H36 O3

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

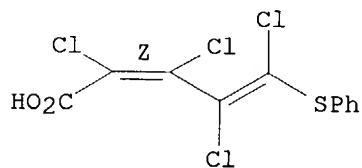
L12 9 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Pentadienoic acid, 5-(acetylphenylamino)-2-cyano- (9CI)
 MF C14 H12 N2 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

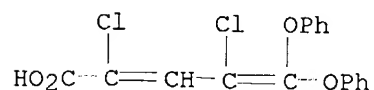
L12 9 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Pentadienoic acid, 2,3,4,5-tetrachloro-5-(phenylthio)-, (?Z)- (9CI)
 MF C11 H6 Cl4 O2 S

Double bond geometry as described by E or Z.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

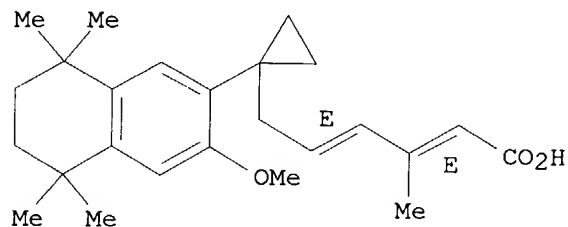
L12 9 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Pentadienoic acid, 2,4-dichloro-5-oxo-, diphenyl acetal (8CI)
 MF C17 H12 Cl2 O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L12 9 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2,4-Hexadienoic acid, 3-methyl-6-[1-(5,6,7,8-tetrahydro-3-methoxy-5,5,8,8-tetramethyl-2-naphthalenyl)cyclopropyl]-, (2E,4E)- (9CI)
MF C25 H34 O3

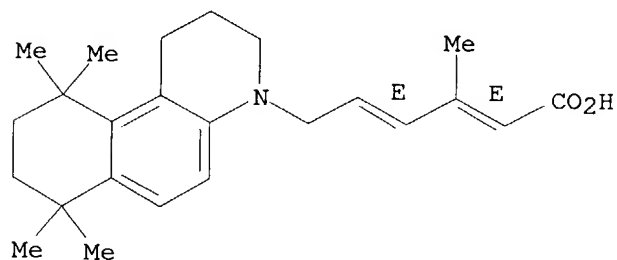
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

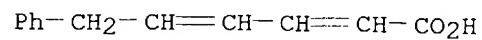
L12 9 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2,4-Hexadienoic acid, 6-(2,3,7,8,9,10-hexahydro-7,7,10,10-tetramethylbenzo[f]quinolin-4(1H)-yl)-3-methyl-, (2E,4E)- (9CI)
MF C24 H33 N O2

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L12 9 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2,4-Hexadienoic acid, 6-phenyl- (9CI)
MF C12 H12 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> e 2,4-Pentadienoic acid, 5-(methylphenylamino)-, (E,Z)-/CN

E1	1	2,4-PENTADIENOIC ACID, 5-(METHYL(2-((2-METHYL-1-OXO-2-PROPENYL)OXY)ETHYL)AMINO)-2-(PHENYLSULFONYL)-, ETHYL ESTER, POLYMER WITH METHYL 2-METHYL-2-PROPENOATE/CN
E2	1	2,4-PENTADIENOIC ACID, 5-(METHYLCARBAMOYL)-, ETHYL ESTER, (Z,Z)-/CN
E3	1 -->	2,4-PENTADIENOIC ACID, 5-(METHYLPHENYLAMINO)-, (E,Z)-/CN
E4	1	2,4-PENTADIENOIC ACID, 5-(METHYLSULFONYL)-, METHYL ESTER, (E,E)-/CN
E5	1	2,4-PENTADIENOIC ACID, 5-(METHYLTHIO)-, METHYL ESTER, (E,E)-/CN
E6	1	2,4-PENTADIENOIC ACID, 5-(METHYLTHIO)-, METHYL ESTER, (Z,E)-/CN
E7	1	2,4-PENTADIENOIC ACID, 5-(O-AMINOPHENYL)-/CN
E8	1	2,4-PENTADIENOIC ACID, 5-(O-AMINOPHENYL)-2-(2-HYDROXYETHYL)-, Γ -LACTONE/CN
E9	1	2,4-PENTADIENOIC ACID, 5-(O-AMINOPHENYL)-2-(O-METHOXYPHENYL)-, ETHYL ESTER/CN
E10	1	2,4-PENTADIENOIC ACID, 5-(O-CHLOROPHENYL)-/CN
E11	1	2,4-PENTADIENOIC ACID, 5-(O-CHLOROPHENYL)-, (E,E)-/CN
E12	1	2,4-PENTADIENOIC ACID, 5-(O-CHLOROPHENYL)-2-(ETHYLSULFONYL)-/CN

=> e7

L13 1 "2,4-PENTADIENOIC ACID, 5-(O-AMINOPHENYL)-"/CN

=> e3

L14 1 "2,4-PENTADIENOIC ACID, 5-(METHYLPHENYLAMINO)-, (E,Z)-"/CN

=> d 114

L14 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN

RN 52331-39-2 REGISTRY

CN **2,4-Pentadienoic acid, 5-(methylphenylamino)-, (E,Z)- (9CI)** (CA INDEX NAME)

FS STEREOSEARCH

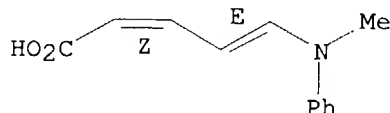
MF C12 H13 N O2

LC STN Files: CA, CAPLUS

DT.CA Cplus document type: Journal

RL.NP Roles from non-patents: RACT (Reactant or reagent)

Double bond geometry as shown.

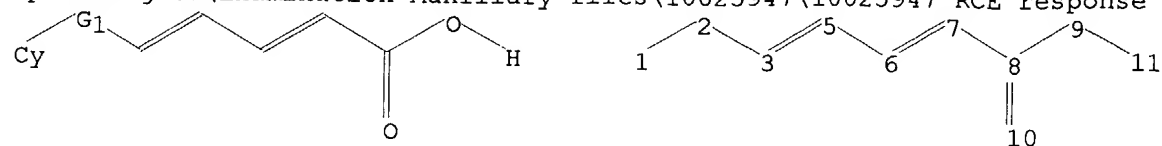


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=>
Uploading C:\Examination Auxillary files\10025947\10025947 RCE response 2nd stab.str



chain nodes :
1 2 3 5 6 7 8 9 10 11
chain bonds :
1-2 2-3 3-5 5-6 6-7 7-8 8-9 8-10 9-11
exact/norm bonds :
1-2 2-3
exact bonds :
3-5 5-6 6-7 7-8 9-11
normalized bonds :
8-9 8-10

G1:S,N,O

Match level :

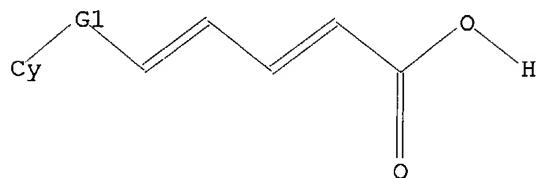
1:Atom 2:CLASS 3:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS

L15 STRUCTURE UPLOADED

=> d l15

L15 HAS NO ANSWERS

L15 STR



G1 S,N,O

Structure attributes must be viewed using STN Express query preparation.

=> search l15 sss sam

SAMPLE SEARCH INITIATED 07:25:58 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 379 TO ITERATE

100.0% PROCESSED 379 ITERATIONS

SEARCH TIME: 00.00.01

4 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 6412 TO 8748

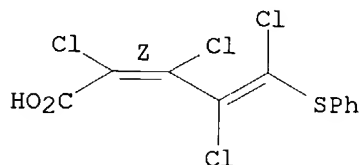
PROJECTED ANSWERS: 4 TO 200

L16 4 SEA SSS SAM L15

=> d scan

L16 4 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2,4-Pentadienoic acid, 2,3,4,5-tetrachloro-5-(phenylthio)-, (?Z)- (9CI)
MF C11 H6 Cl4 O2 S

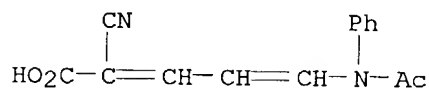
Double bond geometry as described by E or Z.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

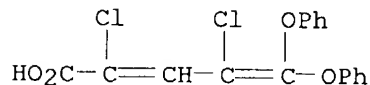
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):4

L16 4 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2,4-Pentadienoic acid, 5-(acetylphenylamino)-2-cyano- (9CI)
MF C14 H12 N2 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

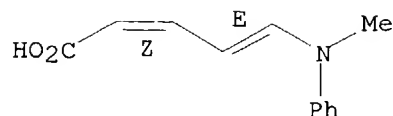
L16 4 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2,4-Pentadienoic acid, 2,4-dichloro-5-oxo-, diphenyl acetal (8CI)
MF C17 H12 Cl2 O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L16 4 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2,4-Pentadienoic acid, 5-(methylphenylamino)-, (E,Z)- (9CI)
MF C12 H13 N O2

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> e2,4-Pentadienoic acid, 5-(methylphenylamino)-, (E,Z)- /cn
'E' NOT FOUND

The E# entered is not currently defined.

=> e 2,4-Pentadienoic acid, 5-(methylphenylamino)-, (E,Z)- /cn

E1	1	2,4-PENTADIENOIC ACID, 5-(METHYL(2-(2-METHYL-1-OXO-2-PROPENYL)OXY)ETHYL)AMINO)-2-(PHENYLSULFONYL)-, ETHYL ESTER, POLYMER WITH METHYL 2-METHYL-2-PROPENOATE/CN
E2	1	2,4-PENTADIENOIC ACID, 5-(METHYLCARBAMOYL)-, ETHYL ESTER, (Z,Z)-/CN
E3	1 -->	2,4-PENTADIENOIC ACID, 5-(METHYLPHENYLAMINO)-, (E,Z)-/CN
E4	1	2,4-PENTADIENOIC ACID, 5-(METHYLSULFONYL)-, METHYL ESTER, (E,E)-/CN
E5	1	2,4-PENTADIENOIC ACID, 5-(METHYLTHIO)-, METHYL ESTER, (E,E)-/CN
E6	1	2,4-PENTADIENOIC ACID, 5-(METHYLTHIO)-, METHYL ESTER, (Z,E)-/CN
E7	1	2,4-PENTADIENOIC ACID, 5-(O-AMINOPHENYL)-/CN
E8	1	2,4-PENTADIENOIC ACID, 5-(O-AMINOPHENYL)-2-(2-HYDROXYETHYL)-, LACTONE/CN
E9	1	2,4-PENTADIENOIC ACID, 5-(O-AMINOPHENYL)-2-(O-METHOXYPHENYL)-, ETHYL ESTER/CN
E10	1	2,4-PENTADIENOIC ACID, 5-(O-CHLOROPHENYL)-/CN
E11	1	2,4-PENTADIENOIC ACID, 5-(O-CHLOROPHENYL)-, (E,E)-/CN
E12	1	2,4-PENTADIENOIC ACID, 5-(O-CHLOROPHENYL)-2-(ETHYLSULFONYL)-/CN

=> e3

L17 1 "2,4-PENTADIENOIC ACID, 5-(METHYLPHENYLAMINO)-, (E,Z)-"/CN

=> d 117

L17 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN

RN 52331-39-2 REGISTRY

CN **2,4-Pentadienoic acid, 5-(methylphenylamino)-, (E,Z)- (9CI)** (CA INDEX NAME)

FS STEREOSEARCH

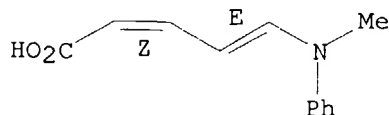
MF C12 H13 N O2

LC STN Files: CA, CAPLUS

DT.CA Caplus document type: Journal

RL.NP Roles from non-patents: RACT (Reactant or reagent)

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> filecaplus

0 FILECAPLUS
L18 0 FILECAPLUS

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	31.34	69.15
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.10

FILE 'CAPLUS' ENTERED AT 07:28:43 ON 19 NOV 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 19 Nov 2004 VOL 141 ISS 21
FILE LAST UPDATED: 17 Nov 2004 (20041117/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> 117

L19 1 L17

=> d 119

L19 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1974:425306 CAPLUS
DN 81:25306
TI Synthesis and thermal splitting of 2-phenyl-6-(4-phenylmethylaminobutadien-1-yl)fulvene
AU Porshnev, Yu. N.; Tereshchenko, E. M.; Churkina, V. A.
CS Nauchno-Issled. Inst. Org. Poluprod. Krasitelei, Moscow, USSR
SO Zhurnal Organicheskoi Khimii (1974), 10(4), 881
CODEN: ZORKAE; ISSN: 0514-7492
DT Journal
LA Russian

=> d 119 ti fbib abs

L19 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN
TI Synthesis and thermal splitting of 2-phenyl-6-(4-phenylmethylaminobutadien-1-yl)fulvene
AN 1974:425306 CAPLUS
DN 81:25306
TI Synthesis and thermal splitting of 2-phenyl-6-(4-phenylmethylaminobutadien-1-yl)fulvene
AU Porshnev, Yu. N.; Tereshchenko, E. M.; Churkina, V. A.
CS Nauchno-Issled. Inst. Org. Poluprod. Krasitelei, Moscow, USSR
SO Zhurnal Organicheskoi Khimii (1974), 10(4), 881
CODEN: ZORKAE; ISSN: 0514-7492
DT Journal
LA Russian
GI For diagram(s), see printed CA Issue.
AB Condensation of Na 1-phenylcyclo-pentadienide with PhNMeCH:CHCH:CHCHO gave a mixture of anti-(I) and syn-fulvenes (II), containing 2% 2-phenylazulene. 1-Phenylazulene was not present in the products, which was explained by the more difficult ring formation from II than I.

=> logoff hold

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	4.05	73.20
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-0.70	-2.80

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 07:29:33 ON 19 NOV 2004

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
SESSION RESUMED IN FILE 'CAPLUS' AT 07:34:02 ON 19 NOV 2004
FILE 'CAPLUS' ENTERED AT 07:34:02 ON 19 NOV 2004
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	4.49	73.64
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-0.70	-2.80

=> file reg

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	4.49	73.64

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.70	-2.80

FILE 'REGISTRY' ENTERED AT 07:34:10 ON 19 NOV 2004
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
 COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 17 NOV 2004 HIGHEST RN 783276-57-3
 DICTIONARY FILE UPDATES: 17 NOV 2004 HIGHEST RN 783276-57-3

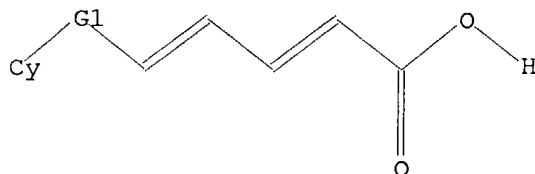
TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> d l11
 L11 HAS NO ANSWERS
 L11 STR



G1 O,S,N,CH2

Structure attributes must be viewed using STN Express query preparation.

=> search l11 sss full
 FULL SEARCH INITIATED 07:34:30 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 8696 TO ITERATE

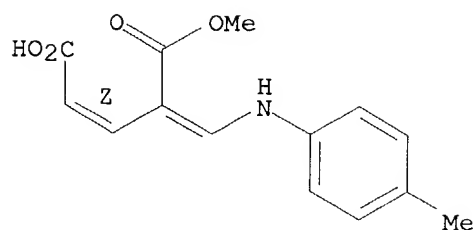
100.0% PROCESSED 8696 ITERATIONS 137 ANSWERS
 SEARCH TIME: 00.00.01

L20 137 SEA SSS FUL L11

=> d scan

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2-Pentenedioic acid, 4-[[[(4-methylphenyl)amino]methylene]-, 5-methyl
 ester, (?Z)- (9CI)
 MF C14 H15 N O4

Double bond geometry as described by E or Z.

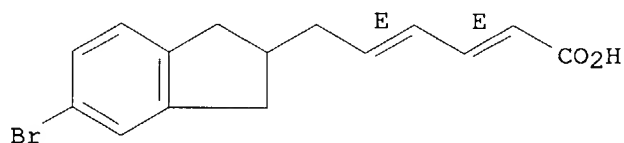


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Hexadienoic acid, 6-(5-bromo-2,3-dihydro-1H-inden-2-yl)-, (E,E)- (9CI)
 MF C15 H15 Br O2

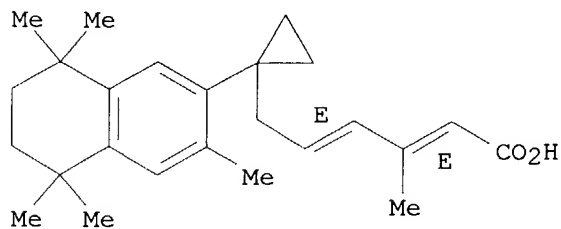
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Hexadienoic acid, 3-methyl-6-[1-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)cyclopropyl]-, (2E,4E)- (9CI)
 MF C25 H34 O2

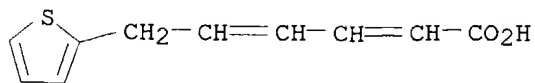
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Hexadienoic acid, 6-(2-thienyl)- (8CI)

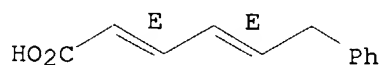
MF C10 H10 O2 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2,4-Hexadienoic acid, 6-phenyl-, (E,E)- (9CI)
MF C12 H12 O2

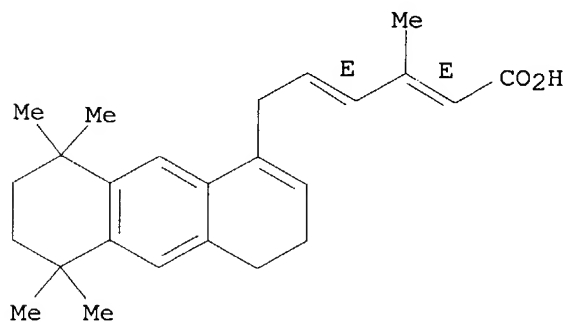
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2,4-Hexadienoic acid, 6-(3,4,5,6,7,8-hexahydro-5,5,8,8-tetramethyl-1-anthracenyl)-3-methyl-, (2E,4E)- (9CI)
MF C25 H32 O2

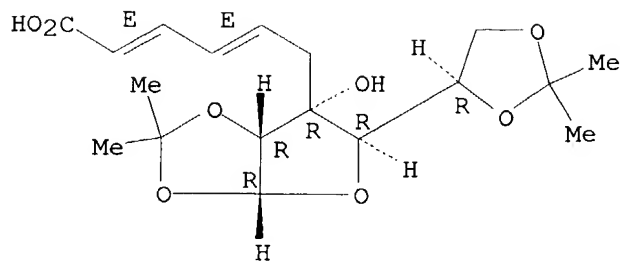
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

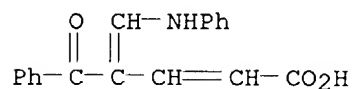
L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN α-D-Allofuranose, 3-C-[(2E,4E)-5-carboxy-2,4-pentadienyl]-1,2:5,6-bis-O-(1-methylethylidene)- (9CI)
MF C18 H26 O8

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



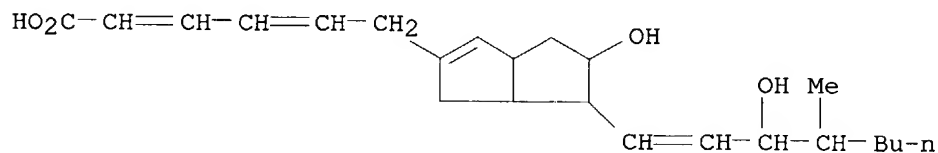
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Pentadienoic acid, 4-benzoyl-5-(phenylamino)- (9CI)
 MF C18 H15 N O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

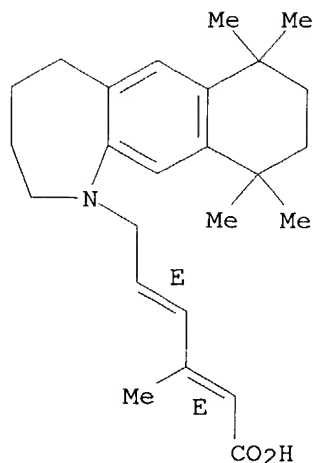
L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Hexadienoic acid, 6-[1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-(3-hydroxy-4-methyl-1-octenyl)-2-pentalenyl]- (9CI)
 MF C23 H34 O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Hexadienoic acid, 3-methyl-6-(2,3,4,5,7,8,9,10-octahydro-7,7,10,10-tetramethyl-1H-naphth[2,3-b]azepin-1-yl)-, (2E,4E)- (9CI)
 MF C25 H35 N O2

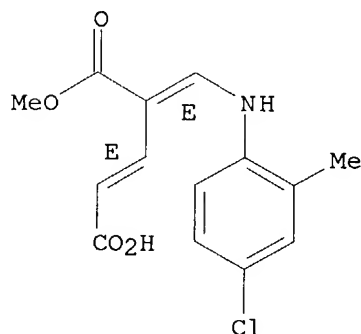
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2-Pentenedioic acid, 4-[[(4-chloro-2-methylphenyl)amino]methylene]-,
 5-methyl ester, (2E,4E)- (9CI)
 MF C14 H14 Cl N O4

Double bond geometry as shown.

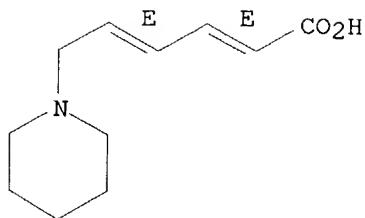


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Hexadienoic acid, 6-(1-piperidinyl)-, hydrochloride, (E,E)- (9CI)
 MF C11 H17 N O2 . Cl H

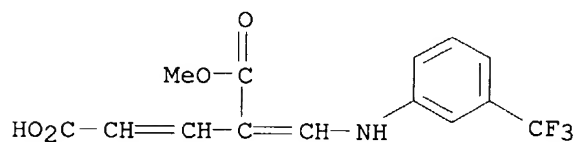
Double bond geometry as shown.



● HCl

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

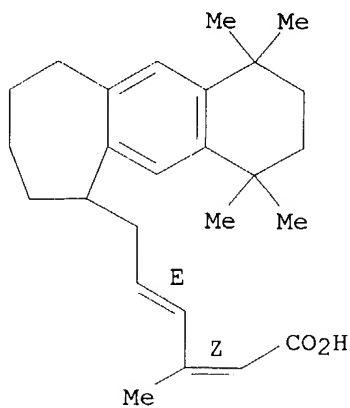
L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2-Pentenedioic acid, 4-[[[3-(trifluoromethyl)phenyl]amino]methylene]-,
 5-methyl ester (9CI)
 MF C14 H12 F3 N O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

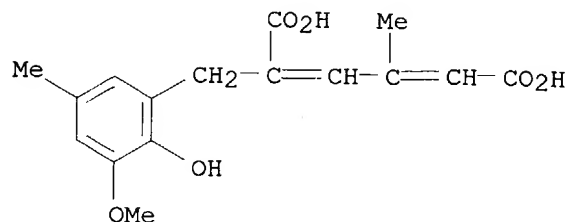
L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Hexadienoic acid, 3-methyl-6-(2,3,4,6,7,8,9,10-octahydro-1,1,4,4-
 tetramethyl-1H-cyclohepta[b]naphthalen-6-yl)-, (2Z,4E)- (9CI)
 MF C26 H36 O2

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

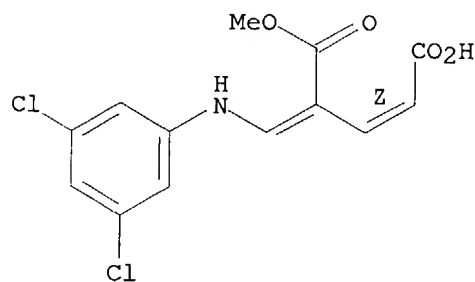
L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2,4-Hexadienedioic acid, 2-[(2-hydroxy-3-methoxy-5-methylphenyl)methyl]-4-methyl- (9CI)
MF C16 H18 O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

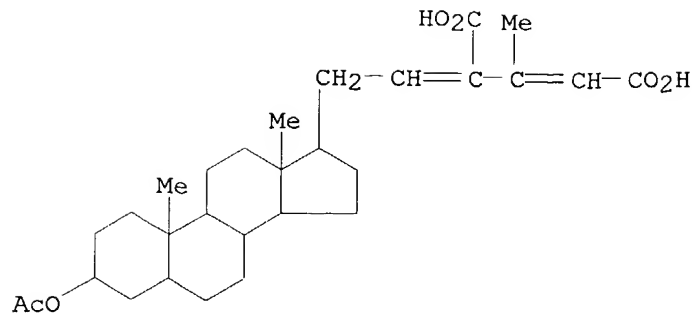
L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2-Pentenedioic acid, 4-[[[(3,5-dichlorophenyl)amino]methylene]-, 5-methyl ester, (? ,Z)- (9CI)
MF C13 H11 Cl2 N O4

Double bond geometry as described by E or Z.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

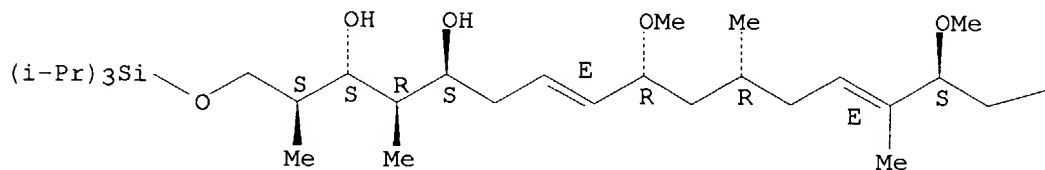
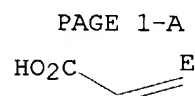
L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2-Pentenedioic acid, 4-[(3 β ,5 β)-3-(acetyloxy)pregnan-21-ylidene]-3-methyl-, (Z,?)- (9CI)
MF C29 H42 O6



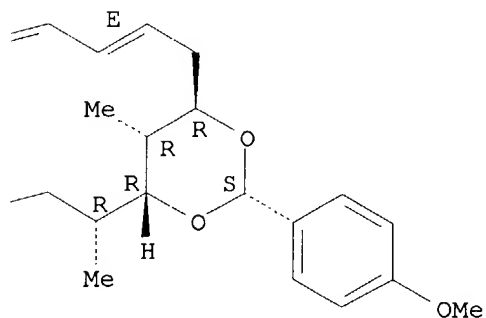
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Hexadienoic acid, 6-[(2S,4R,5R,6R)-6-[(1R,4S,5E,8R,10R,11E,14S,15R,16S,17S)-14,16-dihydroxy-4,10-dimethoxy-1,5,8,15,17-pentamethyl-18-[[tris(1-methylethyl)silyl]oxy]-5,11-octadecadienyl]-2-(4-methoxyphenyl)-5-methyl-1,3-dioxan-4-yl]-, (2E,4E)- (9CI)
 MF C52 H88 O10 Si

Absolute stereochemistry.
 Double bond geometry as shown.

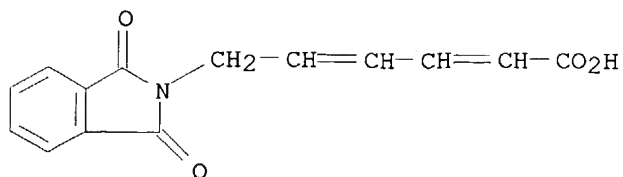


PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

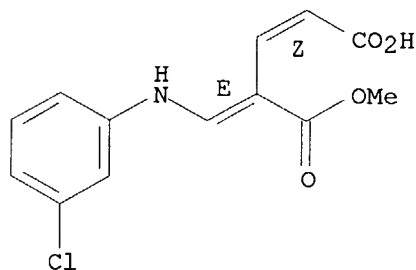
L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2-Isoindolinesorbic acid, 1,3-dioxo- (8CI)
MF C14 H11 N O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2-Pentenedioic acid, 4-[[(3-chlorophenyl)amino]methylene]-, 5-methyl
ester, (E,Z)- (9CI)
MF C13 H12 Cl N O4

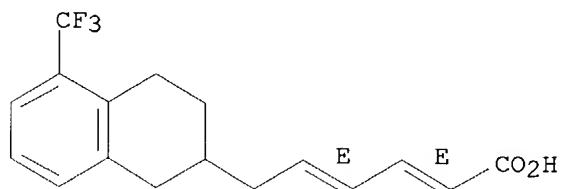
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2,4-Hexadienoic acid, 6-[1,2,3,4-tetrahydro-5-(trifluoromethyl)-2-naphthalenyl]-, (E,E)- (9CI)
MF C17 H17 F3 O2

Double bond geometry as shown.

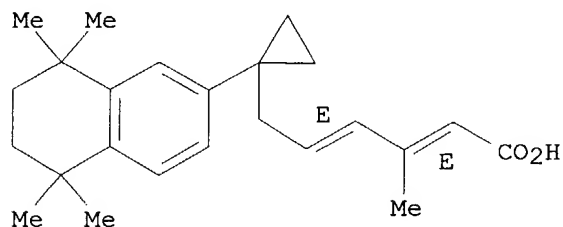


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2,4-Hexadienoic acid, 3-methyl-6-[1-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)cyclopropyl]-, (2E,4E)- (9CI)
MF C24 H32 O2

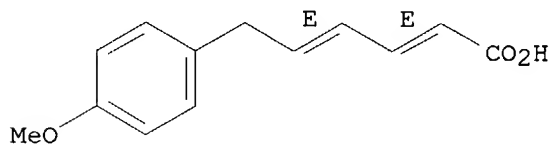
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

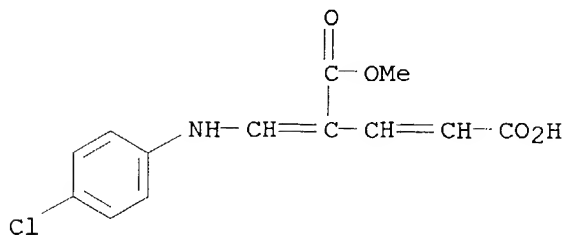
L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2,4-Hexadienoic acid, 6-(4-methoxyphenyl)-, (E,E)- (9CI)
MF C13 H14 O3

Double bond geometry as shown.



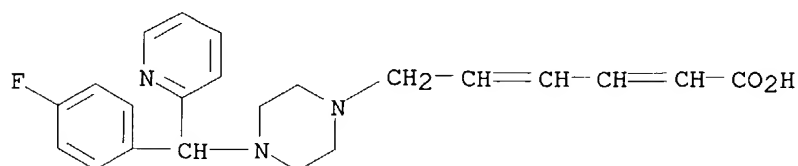
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2-Pentenedioic acid, 4-[[(4-chlorophenyl)amino]methylene]-, 5-methyl ester (9CI)
MF C13 H12 Cl N O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

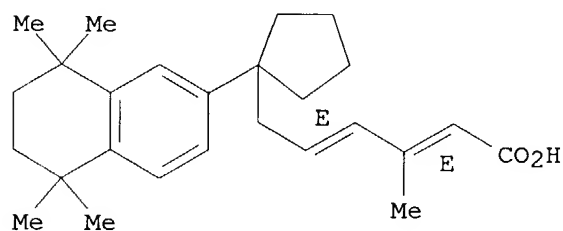
L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Hexadienoic acid, 6-[4-[(4-fluorophenyl)-2-pyridinylmethyl]-1-piperazinyl]-, dihydrochloride (9CI)
 MF C22 H24 F N3 O2 . 2 Cl H



● 2 HCl

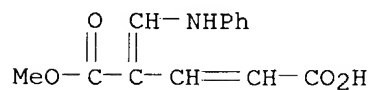
L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Hexadienoic acid, 3-methyl-6-[1-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)cyclopentyl]-, (2E,4E)- (9CI)
 MF C26 H36 O2

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

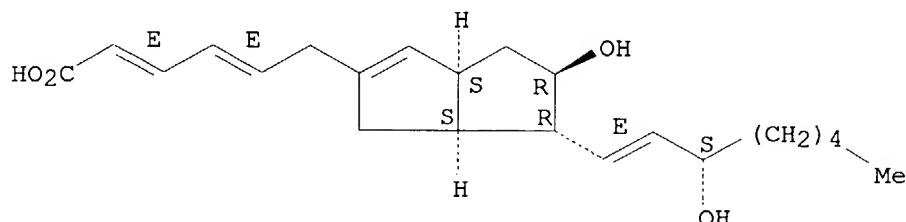
L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2-Pentenedioic acid, 4-[(phenylamino)methylene]-, 5-methyl ester (9CI)
 MF C13 H13 N O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Hexadienoic acid, 6-[1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-(3-hydroxy-1-octenyl)-2-pentalenyl]-, [3aS-[2(2E,4E),3a α ,5 β ,6 α (1E,3R*)
 ,6a α]]- (9CI)
 MF C22 H32 O4

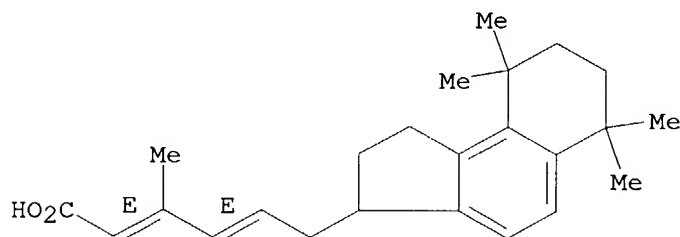
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Hexadienoic acid, 6-(2,3,6,7,8,9-hexahydro-6,6,9,9-tetramethyl-1H-benz[e]inden-3-yl)-3-methyl-, (2E,4E)- (9CI)
 MF C24 H32 O2

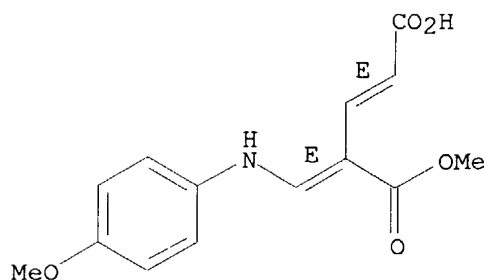
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

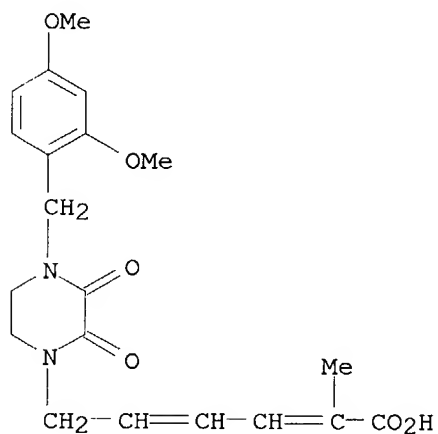
L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2-Pentenedioic acid, 4-[[(4-methoxyphenyl)amino]methylene]-, 5-methyl ester, (2E,4E)- (9CI)
 MF C14 H15 N O5

Double bond geometry as shown.



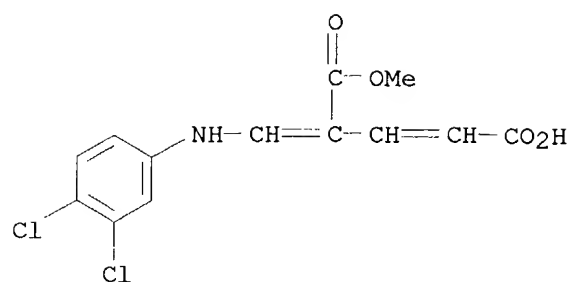
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Hexadienoic acid, 6-[4-[(2,4-dimethoxyphenyl)methyl]-2,3-dioxo-1-piperazinyl]-2-methyl- (9CI)
 MF C20 H24 N2 O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

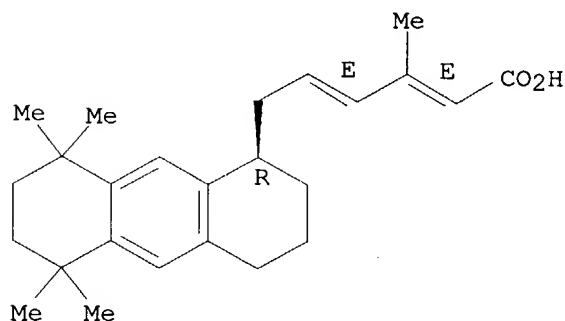
L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2-Pentenedioic acid, 4-[[[(3,4-dichlorophenyl)amino]methylene]-, 5-methyl ester (9CI)
 MF C13 H11 Cl2 N O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Hexadienoic acid, 3-methyl-6-[(1R)-1,2,3,4,5,6,7,8-octahydro-5,5,8,8-tetramethyl-1-anthracenyl]-, (2E,4E)-(+)-(9CI)
 MF C25 H34 O2

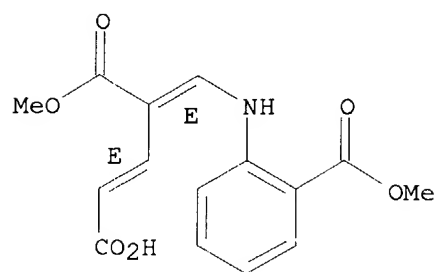
Absolute stereochemistry. Rotation (+).
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2-Pentenedioic acid, 4-[[[2-(methoxycarbonyl)phenyl]amino]methylene]-, 5-methyl ester, (2E,4E)-(9CI)
 MF C15 H15 N O6

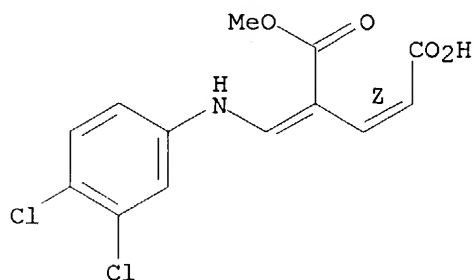
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2-Pentenedioic acid, 4-[[(3,4-dichlorophenyl)amino]methylene]-, 5-methyl
 ester, (? ,Z)- (9CI)
 MF C13 H11 Cl2 N O4

Double bond geometry as described by E or Z.

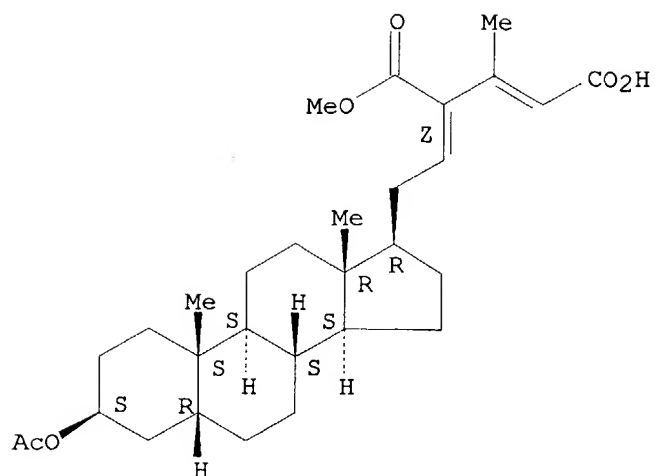


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2-Pentenedioic acid, 4-[(3β,5β)-3-(acetyloxy)pregnan-21-ylidene]-
 3-methyl-, 5-methyl ester, (? ,Z)- (9CI)
 MF C30 H44 O6

Absolute stereochemistry.

Double bond geometry as described by E or Z.

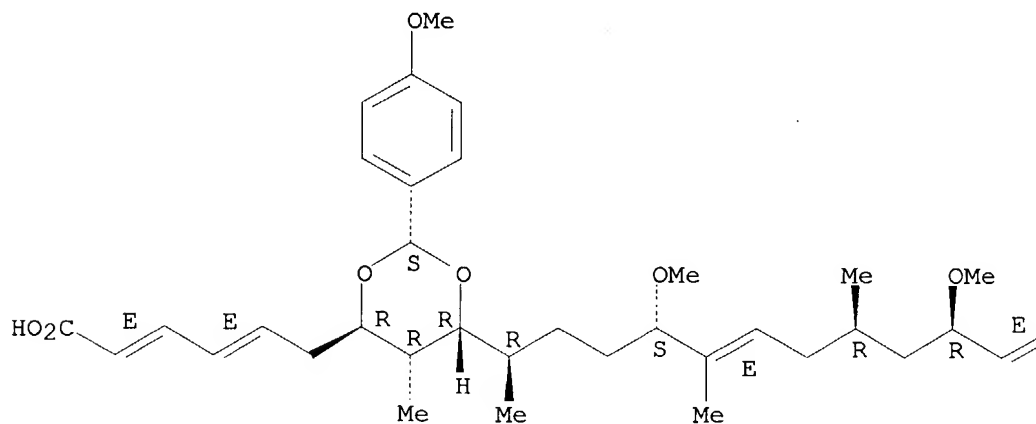


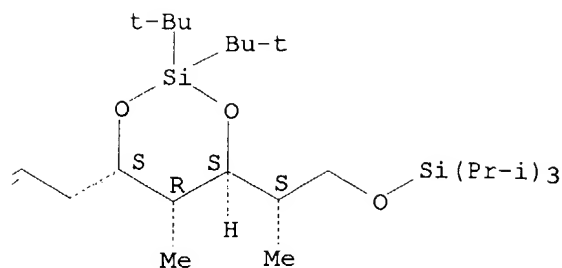
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Hexadienoic acid, 6-[(2S,4R,5R,6R)-6-[(1R,4S,5E,8R,10R,11E)-13-
 [(4S,5R,6S)-2,2-bis(1,1-dimethylethyl)-5-methyl-6-[(1S)-1-methyl-2-
 [[tris(1-methylethyl)silyl]oxy]ethyl]-1,3-dioxo-2-silacyclohex-4-yl]-4,10-
 dimethoxy-1,5,8-trimethyl-5,11-tridecadienyl]-2-(4-methoxyphenyl)-5-methyl-
 1,3-dioxan-4-yl]-, (2E,4E)- (9CI)
 MF C60 H104 O10 Si2

Absolute stereochemistry.
 Double bond geometry as shown.

PAGE 1-A

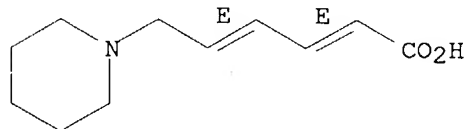




PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Hexadienoic acid, 6-(1-piperidiny1)-, (E,E)- (9CI)
 MF C11 H17 N O2
 CI COM

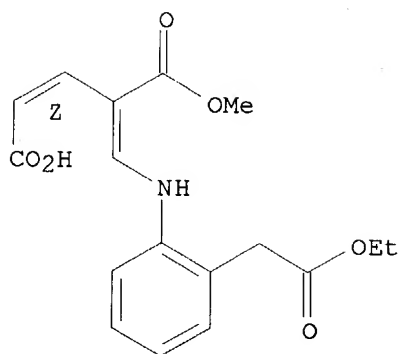
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

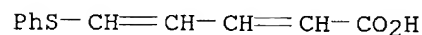
L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2-Pentenedioic acid, 4-[[[2-(2-ethoxy-2-oxoethyl)phenyl]amino]methylene]-, 5-methyl ester, (? ,Z)- (9CI)
 MF C17 H19 N O6

Double bond geometry as described by E or Z.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

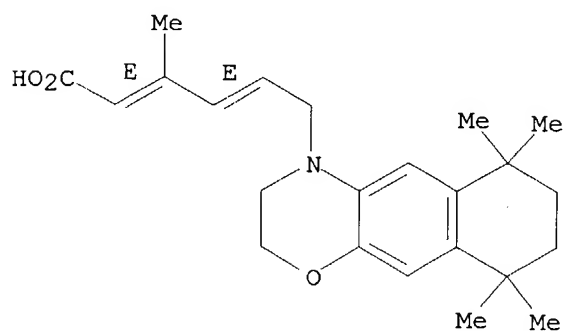
L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Pentadienoic acid, 5-(phenylthio)- (9CI)
 MF C11 H10 O2 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Hexadienoic acid, 6-(2,3,6,7,8,9-hexahydro-6,6,9,9-tetramethyl-4H-naphth[2,3-b]-1,4-oxazin-4-yl)-3-methyl-, (2E,4E)- (9CI)
 MF C23 H31 N O3

Double bond geometry as shown.

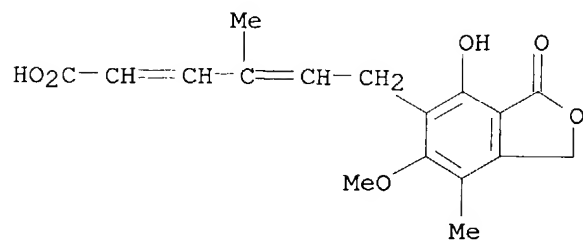


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

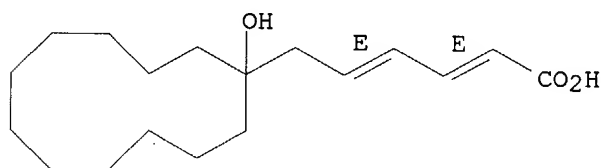
IN 5-Phthalansorbic acid, 4-hydroxy-6-methoxy- γ ,7-dimethyl-3-oxo- (8CI)
 MF C17 H18 O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Hexadienoic acid, 6-(1-hydroxycyclododecyl)-, (E,E)- (9CI)
 MF C18 H30 O3

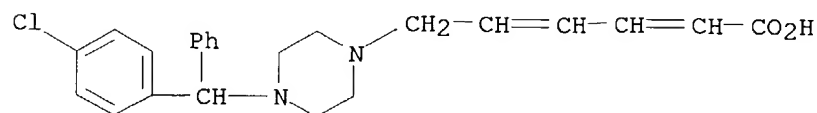
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

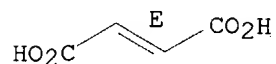
L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Hexadienoic acid, 6-[4-[(4-chlorophenyl)phenylmethyl]-1-piperazinyl]-, (2E)-2-butenedioate (1:1) (9CI)
 MF C23 H25 Cl N2 O2 . C4 H4 O4

CM 1



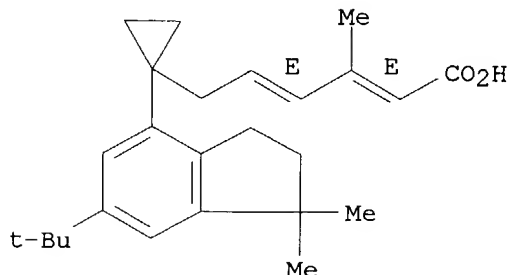
CM 2

Double bond geometry as shown.



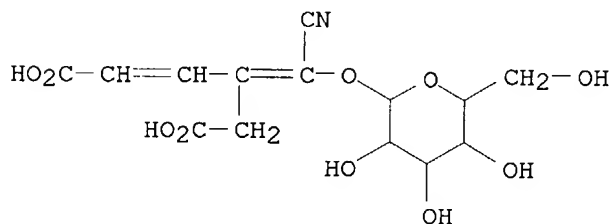
L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Hexadienoic acid, 6-[1-[6-(1,1-dimethylethyl)-2,3-dihydro-1,1-dimethyl-1H-inden-4-yl]cyclopropyl]-3-methyl-, (2E,4E)- (9CI)
 MF C25 H34 O2

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

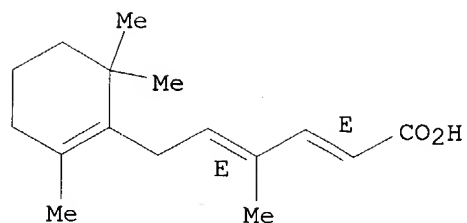
L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2-Hexenedioic acid, 4-[cyano(β-D-glucopyranosyloxy)methylene]-, (2E,4E)- (9CI)
 MF C14 H17 N O10



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 1-Cyclohexene-1-sorbic acid, γ,2,6,6-tetramethyl- (6CI)
 MF C16 H24 O2

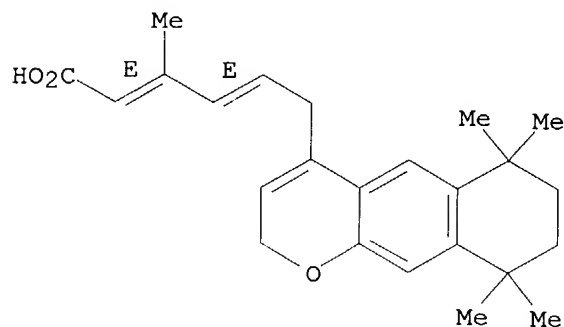
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Hexadienoic acid, 3-methyl-6-(6,7,8,9-tetrahydro-6,6,9,9-tetramethyl-
 2H-naphtho[2,3-b]pyran-4-yl)-, (2E,4E)- (9CI)
 MF C24 H30 O3

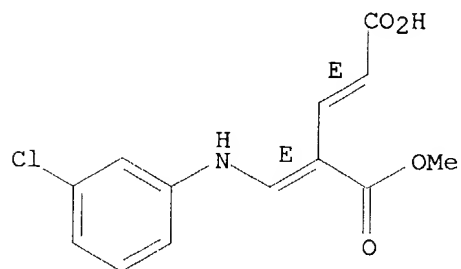
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

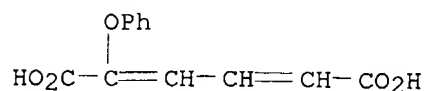
L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2-Pentenedioic acid, 4-[[[(3-chlorophenyl)amino]methylene]-, 5-methyl
 ester, (2E,4E)- (9CI)
 MF C13 H12 Cl N O4

Double bond geometry as shown.



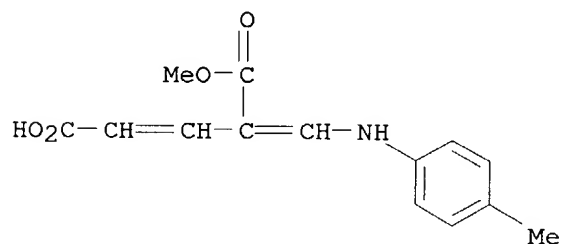
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2,4-Hexadienedioic acid, 2-phenoxy- (9CI)
MF C12 H10 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

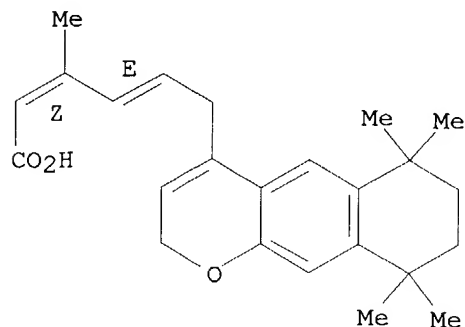
L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2-Pentenedioic acid, 4-[[(4-methylphenyl) amino]methylene]-, 5-methyl ester (9CI)
MF C14 H15 N O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2,4-Hexadienoic acid, 3-methyl-6-(6,7,8,9-tetrahydro-6,6,9,9-tetramethyl-2H-naphtho[2,3-b]pyran-4-yl)-, (2Z,4E)- (9CI)
MF C24 H30 O3

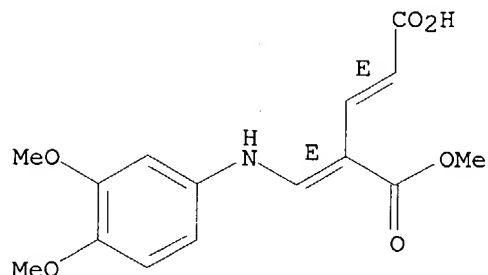
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2-Pentenedioic acid, 4-[[(3,4-dimethoxyphenyl)amino]methylene]-, 5-methyl
ester, (2E,4E)- (9CI)
MF C15 H17 N O6

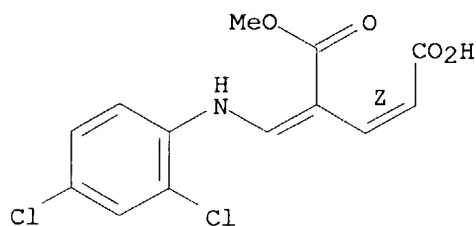
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2-Pentenedioic acid, 4-[[(2,4-dichlorophenyl)amino]methylene]-, 5-methyl
ester, (? ,Z)- (9CI)
MF C13 H11 Cl2 N O4

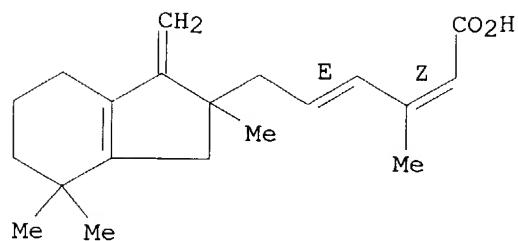
Double bond geometry as described by E or Z.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2,4-Hexadienoic acid, 6-(2,3,4,5,6,7-hexahydro-2,4,4-trimethyl-1-methylene-1H-inden-2-yl)-3-methyl-, (Z,E)- (9CI)
MF C20 H28 O2

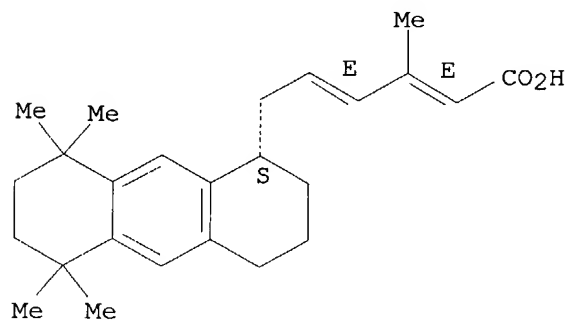
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

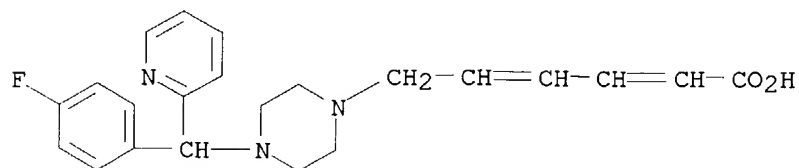
L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Hexadienoic acid, 3-methyl-6-[(1S)-1,2,3,4,5,6,7,8-octahydro-5,5,8,8-tetramethyl-1-anthracenyl]-, (2E,4E)-(-)-(9CI)
 MF C25 H34 O2

Absolute stereochemistry. Rotation (-).
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

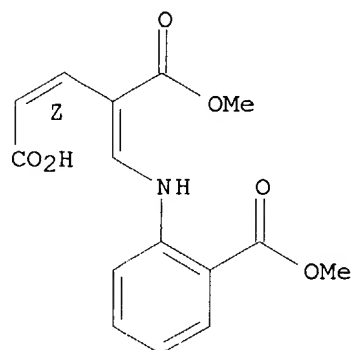
L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Hexadienoic acid, 6-[4-[(4-fluorophenyl)-2-pyridinylmethyl]-1-piperazinyl]- (9CI)
 MF C22 H24 F N3 O2
 CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2-Pentenedioic acid, 4-[[[2-(methoxycarbonyl)phenyl]amino]methylene]-,
 5-methyl ester, (? ,Z)- (9CI)
 MF C15 H15 N O6

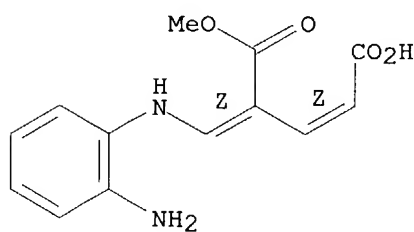
Double bond geometry as described by E or Z.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2-Pentenedioic acid, 4-[[[2-aminophenyl]amino]methylene]-, 5-methyl ester,
 (Z,Z)- (9CI)
 MF C13 H14 N2 O4

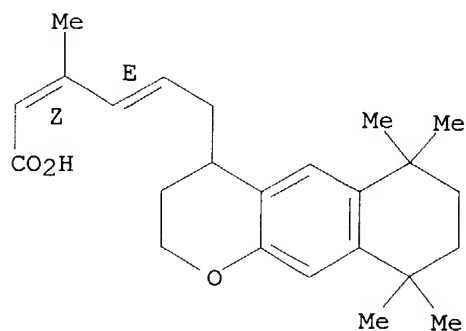
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

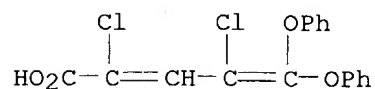
L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Hexadienoic acid, 6-(3,4,6,7,8,9-hexahydro-6,6,9,9-tetramethyl-2H-
 naphtho[2,3-b]pyran-4-yl)-3-methyl-, (2Z,4E)- (9CI)
 MF C24 H32 O3

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Pentadienoic acid, 2,4-dichloro-5-oxo-, diphenyl acetal (8CI)
 MF C17 H12 Cl2 O4

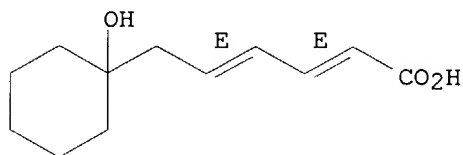


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

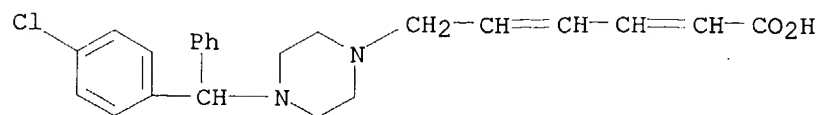
L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Hexadienoic acid, 6-(1-hydroxycyclohexyl)-, (E,E)- (9CI)
 MF C12 H18 O3

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

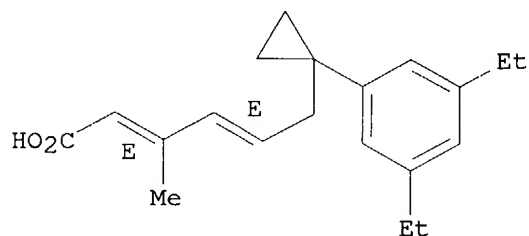
L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Hexadienoic acid, 6-[4-[(4-chlorophenyl)phenylmethyl]-1-piperazinyl]-
 (9CI)
 MF C23 H25 Cl N2 O2
 CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

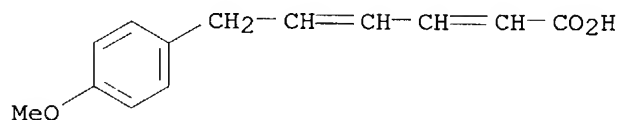
L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Hexadienoic acid, 6-[1-(3,5-diethylphenyl)cyclopropyl]-3-methyl-,
 (2E,4E)- (9CI)
 MF C20 H26 O2

Double bond geometry as shown.



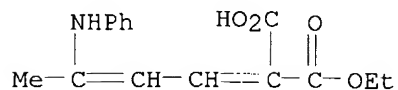
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Hexadienoic acid, 6-(4-methoxyphenyl)- (9CI)
 MF C13 H14 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

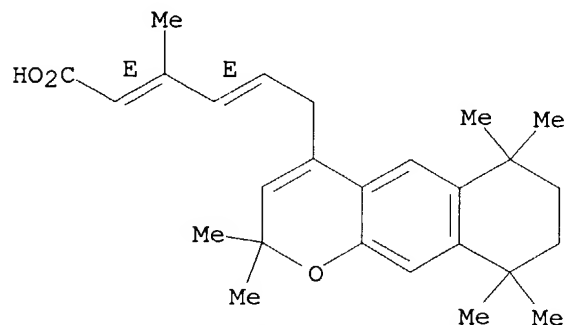
L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Malonic acid, (3-anilino-2-butenylidene)-, ethyl ester (6CI)
 MF C15 H17 N O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2,4-Hexadienoic acid, 3-methyl-6-(6,7,8,9-tetrahydro-2,2,6,6,9,9-hexamethyl-2H-naphtho[2,3-b]pyran-4-yl)-, (2E,4E)- (9CI)
MF C26 H34 O3

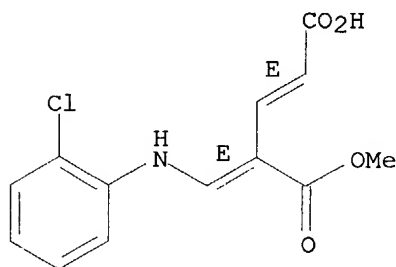
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2-Pentenedioic acid, 4-[[(2-chlorophenyl)amino]methylene]-, 5-methyl ester, (2E,4E)- (9CI)
MF C13 H12 Cl N O4

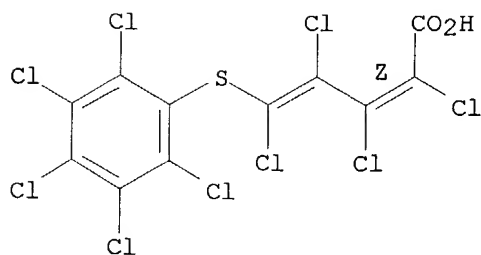
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

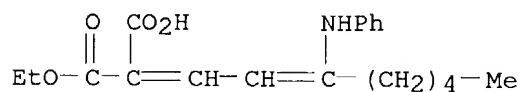
L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2,4-Pentadienoic acid, 2,3,4,5-tetrachloro-5-[(pentachlorophenyl)thio]-, (? ,Z)- (9CI)
MF C11 H Cl9 O2 S

Double bond geometry as described by E or Z.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

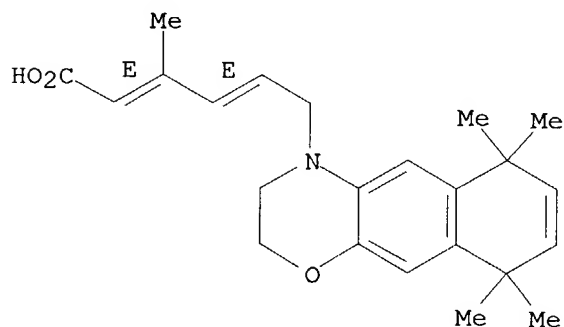
L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Malonic acid, (3-anilino-2-octenylidene)-, ethyl ester (6CI)
 MF C19 H25 N O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Hexadienoic acid, 3-methyl-6-(2,3,6,9-tetrahydro-6,6,9,9-tetramethyl-4H-naphth[2,3-b]-1,4-oxazin-4-yl)-, (2E,4E)- (9CI)
 MF C23 H29 N O3

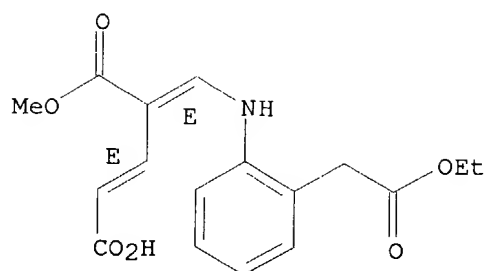
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2-Pentenedioic acid, 4-[[[2-(2-ethoxy-2-oxoethyl)phenyl]amino]methylene]-, 5-methyl ester, (2E,4E)- (9CI)
 MF C17 H19 N O6

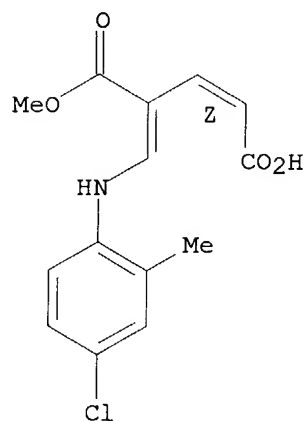
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2-Pentenedioic acid, 4-[[[4-chloro-2-methylphenyl]amino]methylene]-,
 5-methyl ester, (? ,Z)- (9CI)
 MF C14 H14 Cl N O4

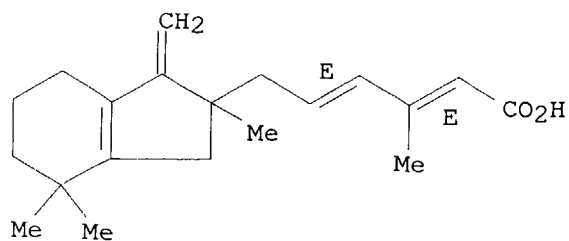
Double bond geometry as described by E or Z.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Hexadienoic acid, 6-(2,3,4,5,6,7-hexahydro-2,4,4-trimethyl-1-methylene-
 1H-inden-2-yl)-3-methyl-, (E,E)- (9CI)
 MF C20 H28 O2

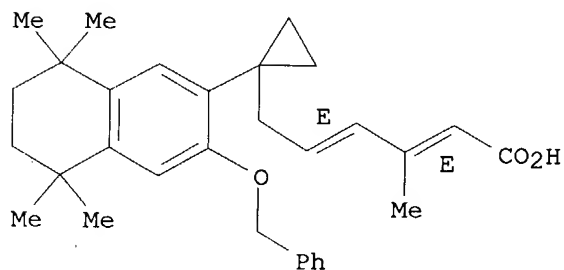
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Hexadienoic acid, 3-methyl-6-[1-[5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-3-(phenylmethoxy)-2-naphthalenyl]cyclopropyl]-, (E,E)- (9CI)
 MF C31 H38 O3

Double bond geometry as shown.

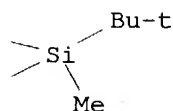
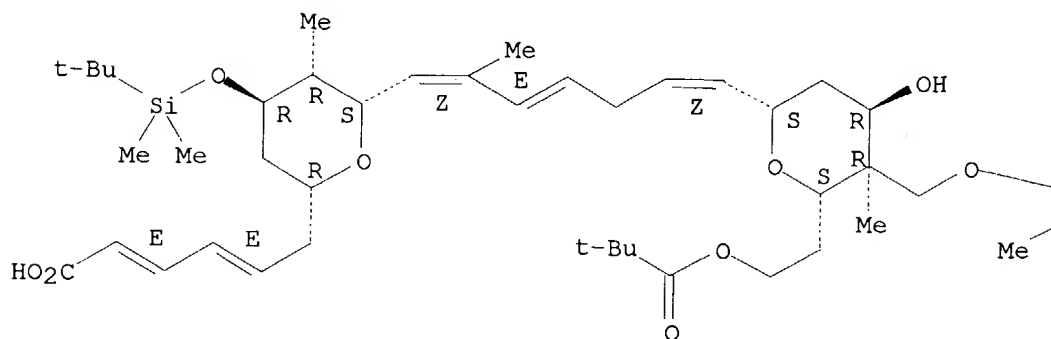


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Hexadienoic acid, 6-[(2R,4R,5R,6S)-4-[[[1,1-dimethylethyl]dimethylsilyl]oxy]-6-[(1Z,3E,6Z)-7-[(2S,4R,5R,6S)-5-[[[1,1-dimethylethyl]dimethylsilyl]oxy]methyl]-6-[2-(2,2-dimethyl-1-oxopropoxy)ethyl]tetrahydro-4-hydroxy-5-methyl-2H-pyran-2-yl]-2-methyl-1,3,6-heptatrienyl]tetrahydro-5-methyl-2H-pyran-2-yl]-, (2E,4E)- (9CI)
 MF C46 H80 O9 Si2

Absolute stereochemistry.

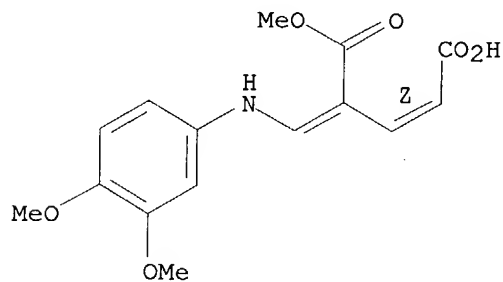
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2-Pentenedioic acid, 4-[[[(3,4-dimethoxyphenyl)amino]methylene]-, 5-methyl
 ester, (? ,Z)- (9CI)
 MF C15 H17 N O6

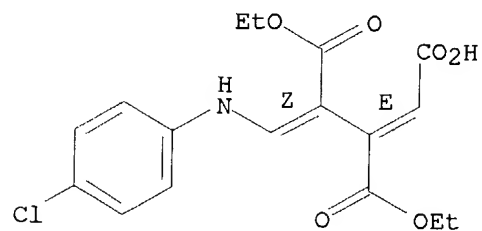
Double bond geometry as described by E or Z.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 1,3-Butadiene-1,2,3-tricarboxylic acid, 4-[(4-chlorophenyl)amino]-,
 2,3-diethyl ester, (Z,E)- (9CI)
 MF C17 H18 Cl N O6

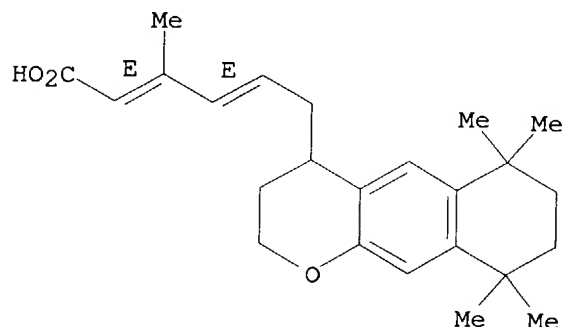
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

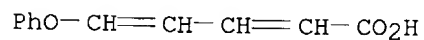
L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Hexadienoic acid, 6-(3,4,6,7,8,9-hexahydro-6,6,9,9-tetramethyl-2H-naphtho[2,3-b]pyran-4-yl)-3-methyl-, (2E,4E)- (9CI)
 MF C24 H32 O3

Double bond geometry as shown.



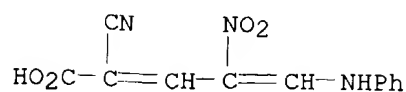
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Pentadienoic acid, 5-phenoxy- (8CI, 9CI)
 MF C11 H10 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 137 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2,4-Pentadienoic acid, 5-anilino-2-cyano-4-nitro-, sodium salt (7CI)
 MF C12 H9 N3 O4 . Na



● Na

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> save temp l20 rawlstab/a

ANSWER SET L20 HAS BEEN SAVED AS 'RAWLISTAB/A'

=> e 2,4-Hexadienoic acid, 6-(1-piperidinyl)-, (E,E)-/cn

E1	1	2,4-HEXADIENOIC ACID, 6-(1-PIPERAZINYL)-, ETHYL ESTER/CN
E2	1	2,4-HEXADIENOIC ACID, 6-(1-PIPERAZINYL)-, ETHYL ESTER, MONOH YDROCHLORIDE/CN
E3	1 -->	2,4-HEXADIENOIC ACID, 6-(1-PIPERIDINYL)-, (E,E)-/CN
E4	1	2,4-HEXADIENOIC ACID, 6-(1-PIPERIDINYL)-, ETHYL ESTER/CN
E5	1	2,4-HEXADIENOIC ACID, 6-(1-PIPERIDINYL)-, ETHYL ESTER, (E,E) -/CN
E6	1	2,4-HEXADIENOIC ACID, 6-(1-PIPERIDINYL)-, ETHYL ESTER, HYDRO CHLORIDE/CN
E7	1	2,4-HEXADIENOIC ACID, 6-(1-PIPERIDINYL)-, HYDROCHLORIDE, (E, E)-/CN
E8	1	2,4-HEXADIENOIC ACID, 6-(10-(ACETYLAMINO)-3,4,5,6,7,8-HEXAHY DRO-5,5,8,8-TETRAMETHYL-1(2H)-ANTHRACENYLIDENE)-3-METHYL-, (2E,4E,6Z)-/CN
E9	1	2,4-HEXADIENOIC ACID, 6-(10-(ACETYLAMINO)-3,4,5,6,7,8-HEXAHY DRO-5,5,8,8-TETRAMETHYL-1(2H)-ANTHRACENYLIDENE)-3-METHYL-, E THYL ESTER, (2E,4E,6Z)-/CN
E10	1	2,4-HEXADIENOIC ACID, 6-(12,15,24-TRIMETHYL-3-OXO-2,22,26-TR IOXATRICYCLO(19.3.1.19,13)HEXACOSA-4,6,11,14,16,19-HEXAEN-23 -YL)-, 5-METHYL-2-METHYLENEHEXYL ESTER, (1R-(1R*,4E,6E,9S*,1 3R*,14Z,16E,19Z,21S*)/CN
E11	1	2,4-HEXADIENOIC ACID, 6-(12,15,24-TRIMETHYL-3-OXO-24-PHENYL- 2,22,26-TRIOXATRICYCLO(19.3.1.19,13)HEXACOSA-4,6,11,14,16,19 -HEXAEN-23-YL)-, 5-METHYL-2-METHYLENEHEXYL ESTER, (1R-(1R*,4 E,6E,9S*,13R*,14Z,16E)/CN
E12	1	2,4-HEXADIENOIC ACID, 6-(1H-PURIN-6-YLTHIO)-/CN

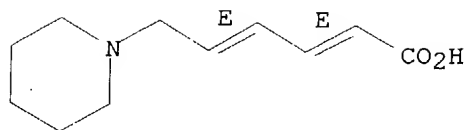
=> e3

L21 1 "2,4-HEXADIENOIC ACID, 6-(1-PIPERIDINYL)-, (E,E)-"/CN

=> d 121

L21 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
 RN 758641-56-4 REGISTRY
 CN **2,4-Hexadienoic acid, 6-(1-piperidinyl)-, (E,E)- (9CI)** (CA
 INDEX NAME)
 FS STEREOSEARCH
 MF C11 H17 N O2
 CI COM
 SR CA

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

```
=> e 2,4-Hexadienoic acid, 6-(1-hydroxycyclododecyl)-, (E,E)-/cn
E1      1      2,4-HEXADIENOIC ACID, 6-(1-ETHYL-2,3,6,7,8,9-HEXAHYDRO-6,6,9
           ,9-TETRAMETHYLBENZO(G)QUINOLIN-4(1H)-YLIDENE)-3-METHYL-, (AL
           L-E)-/CN
E2      1      2,4-HEXADIENOIC ACID, 6-(1-ETHYL-2,3,6,7,8,9-HEXAHYDRO-6,6,9
           ,9-TETRAMETHYLBENZO(G)QUINOLIN-4(1H)-YLIDENE)-3-METHYL-, ETH
           YL ESTER, (2E,4E,6E)-/CN
E3      1 --> 2,4-HEXADIENOIC ACID, 6-(1-HYDROXYCYCLODODECYL)-, (E,E)-/CN
E4      1      2,4-HEXADIENOIC ACID, 6-(1-HYDROXYCYCLODODECYL)-, METHYL EST
           ER, (E,E)-/CN
E5      1      2,4-HEXADIENOIC ACID, 6-(1-HYDROXYCYCLODODECYL)-3-METHYL-, (
           Z,E)-/CN
E6      1      2,4-HEXADIENOIC ACID, 6-(1-HYDROXYCYCLOHEXYL)-, (E,E)-/CN
E7      1      2,4-HEXADIENOIC ACID, 6-(1-HYDROXYCYCLOHEXYL)-, METHYL ESTER
           , (E,E)-/CN
E8      1      2,4-HEXADIENOIC ACID, 6-(1-HYDROXYCYCLOHEXYL)-3-METHYL-, MET
           HYL ESTER, (Z,E)-/CN
E9      1      2,4-HEXADIENOIC ACID, 6-(1-PIPERAZINYL)-, ETHYL ESTER/CN
E10     1      2,4-HEXADIENOIC ACID, 6-(1-PIPERAZINYL)-, ETHYL ESTER, MONOH
           YDROCHLORIDE/CN
E11     1      2,4-HEXADIENOIC ACID, 6-(1-PIPERIDINYL)-, (E,E)-/CN
E12     1      2,4-HEXADIENOIC ACID, 6-(1-PIPERIDINYL)-, ETHYL ESTER/CN
```

=> e3

```
L22      1 "2,4-HEXADIENOIC ACID, 6-(1-HYDROXYCYCLODODECYL)-, (E,E)-"/CN
```

=> d 122

L22 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN

RN 100903-88-6 REGISTRY

CN **2,4-Hexadienoic acid, 6-(1-hydroxycyclododecyl)-, (E,E)- (9CI)**
(CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Cyclododecane, 2,4-hexadienoic acid deriv.

FS STEREOSEARCH

MF C18 H30 O3

SR CA

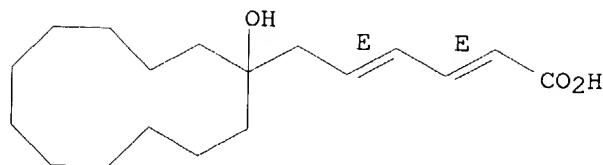
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT

(*File contains numerically searchable property data)

DT.CA CAPLUS document type: Journal

RL.NP Roles from non-patents: PREP (Preparation)

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
172.86	246.50

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-2.80

CA SUBSCRIBER PRICE

FILE 'CAPLUS' ENTERED AT 07:41:58 ON 19 NOV 2004
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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE COVERS 1907 - 19 Nov 2004 VOL 141 ISS 21
FILE LAST UPDATED: 17 Nov 2004 (20041117/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> 122

L23 2 L22

=> d 123 1-2 ti fbib abs

L23 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
TI Unsaturated carboxylic acid polyenolates. Lithium trienolate of sorbic acid as a d6 synthon. Addition to ketones and unsaturated ketones
AN 1989:134699 CAPLUS
DN 110:134699
TI Unsaturated carboxylic acid polyenolates. Lithium trienolate of sorbic acid as a d6 synthon. Addition to ketones and unsaturated ketones
AU Ballester, Pablo; Costa, Antonio; Garcia-Raso, Angel; Mestres, Ramon
CS Dep. Quim., Univ. Illes Balears, Palma de Mallorca, Spain

SO Journal of the Chemical Society, Perkin Transactions 1: Organic and
Bio-Organic Chemistry (1972-1999) (1988), (10), 2797-803
CODEN: JCPRB4; ISSN: 0300-922X
DT Journal
LA English
OS CASREACT 110:134699
AB Lithiated sorbic acid was treated with R1COR2 [R1 = alkyl, Ph; R2 = alkyl,
Ph, alkenyl; R1R2 = (CH2)5, (CH2)11] to give R1CR2C(OH)CH2CH:CHCH:CHCO2H
and CH2:CHCH:CHCH[C(OH)R1R2]CO2H. 2-Cyclohexenone gave
4-(3-oxocyclohexyl)-2,5-hexadienoic acid.

L23 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
TI Lithium trienolate of sorbic acid as a d6 synthon. Synthesis of
7-hydroxy-2,4-dienoic acids
AN 1986:129465 CAPLUS
DN 104:129465
TI Lithium trienolate of sorbic acid as a d6 synthon. Synthesis of
7-hydroxy-2,4-dienoic acids
AU Ballester, P.; Costa, A.; Garcia-Raso, A.; Gomez-Solivellas, A.; Mestres,
R.
CS Dep. Quim. Org., Univ. Palma de Mallorca, Palma de Mallorca, 07071, Spain
SO Tetrahedron Letters (1985), 26(30), 3625-8
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
OS CASREACT 104:129465
AB The trienolate, trans-CH2:CHCH:CHCH:C(OLi)2, of sorbic acid is an easily
available d6 synthon. Preparation of trans,trans-RC(OH)R1CH2CH:CHCH:CHCO2H
from ketones is described.

=> file reg

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	7.74	254.24
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-1.40	-4.20

FILE 'REGISTRY' ENTERED AT 07:45:24 ON 19 NOV 2004
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STRUCTURE FILE UPDATES: 17 NOV 2004 HIGHEST RN 783276-57-3
DICTIONARY FILE UPDATES: 17 NOV 2004 HIGHEST RN 783276-57-3

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> e 2,4-Hexadienoic acid,

6-(1,2,3,4-tetrahydro-5-(trifluoromethyl)-2-naphthalenyl)-, (E,E)-/CN

E1	1	2,4-HEXADIENOIC ACID, 6-(1,2,3,4-TETRAHYDRO-2-NAPHTHALENYL)-, (E,E)-/CN
E2	1	2,4-HEXADIENOIC ACID, 6-(1,2,3,4-TETRAHYDRO-2-NAPHTHALENYL)-, ETHYL ESTER, (E,E)-/CN
E3	1 -->	2,4-HEXADIENOIC ACID, 6-(1,2,3,4-TETRAHYDRO-5-(TRIFLUOROMETHYL)-2-NAPHTHALENYL)-, (E,E)-/CN
E4	1	2,4-HEXADIENOIC ACID, 6-(1,2,3,6,7,8-HEXAHYDRO-1,1,3,3-TETRAMETHYL-5H-BENZ(F)INDEN-5-YLIDENE)-3-METHYL-, (2E,4E,6E)-/CN
E5	1	2,4-HEXADIENOIC ACID, 6-(1,2,3,6,7,8-HEXAHYDRO-1,1,3,3-TETRAMETHYL-5H-BENZ(F)INDEN-5-YLIDENE)-3-METHYL-, (2E,4E,6Z)-/CN
E6	1	2,4-HEXADIENOIC ACID, 6-(1,2,3,6,7,8-HEXAHYDRO-1,1,3,3-TETRAMETHYL-5H-BENZ(F)INDEN-5-YLIDENE)-3-METHYL-, (2Z,4E,6E)-/CN
E7	1	2,4-HEXADIENOIC ACID, 6-(1,2,3,6,7,8-HEXAHYDRO-1,1,3,3-TETRAMETHYL-5H-BENZ(F)INDEN-5-YLIDENE)-3-METHYL-, (ALL-E)-/CN
E8	1	2,4-HEXADIENOIC ACID, 6-(1,2,3,6,7,8-HEXAHYDRO-1,1,3,3-TETRAMETHYL-5H-BENZ(F)INDEN-5-YLIDENE)-3-METHYL-, ETHYL ESTER, (2E,4E,6E)-/CN
E9	1	2,4-HEXADIENOIC ACID, 6-(1,2,3,6,7,8-HEXAHYDRO-1,1,3,3-TETRAMETHYL-5H-BENZ(F)INDEN-5-YLIDENE)-3-METHYL-, ETHYL ESTER, (2E,4E,6Z)-/CN
E10	1	2,4-HEXADIENOIC ACID, 6-(1,2,3,6,7,8-HEXAHYDRO-1,1,3,3-TETRAMETHYL-5H-BENZ(F)INDEN-5-YLIDENE)-3-METHYL-, ETHYL ESTER, (2Z,4E,6E)-/CN
E11	1	2,4-HEXADIENOIC ACID, 6-(1,2,3,6,7,8-HEXAHYDRO-1,1,3,3-TETRAMETHYL-5H-BENZ(F)INDEN-5-YLIDENE)-3-METHYL-, ETHYL ESTER, (ALL-E)-/CN
E12	1	2,4-HEXADIENOIC ACID, 6-(1,2,3,7,8,9-HEXAHYDRO-1,1,3,3-TETRAMETHYL-6H-BENZ(E)INDEN-6-YLIDENE)-3-METHYL-, (2E,4E,6Z)-/CN

=> e3

L24 1 "2,4-HEXADIENOIC ACID, 6-(1,2,3,4-TETRAHYDRO-5-(TRIFLUOROMETHYL)-2-NAPHTHALENYL)-, (E,E)-"/CN

=> d 124

L24 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN

RN 148334-33-2 REGISTRY

CN **2,4-Hexadienoic acid, 6-[1,2,3,4-tetrahydro-5-(trifluoromethyl)-2-naphthalenyl]-, (E,E)- (9CI)** (CA INDEX NAME)

FS STEREOSEARCH

MF C17 H17 F3 O2

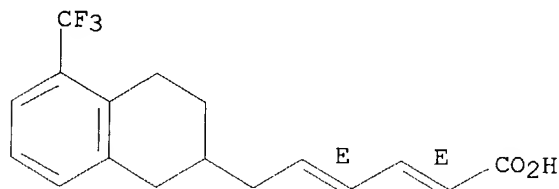
SR CA

LC STN Files: CA, CAPLUS, USPATFULL

DT.CA CAplus document type: Patent

RL.P Roles from patents: PROC (Process)

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
6.62	260.86

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-4.20

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FILE 'CAPLUS' ENTERED AT 07:46:17 ON 19 NOV 2004
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FILE COVERS 1907 - 19 Nov 2004 VOL 141 ISS 21
FILE LAST UPDATED: 17 Nov 2004 (20041117/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> l24

L25 1 L24

=> d l25 ti fbib abs

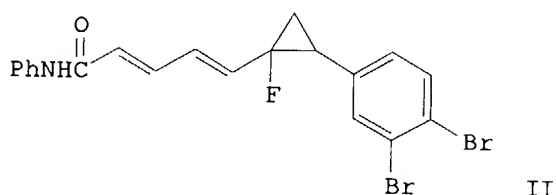
L25 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN
TI Preparation of (phenylcyclopropyl)pentadienamides and analogs as pesticides
AN 1993:603161 CAPLUS
DN 119:203161
TI Preparation of (phenylcyclopropyl)pentadienamides and analogs as pesticides
IN Robinson, John Edward; Cockerill, George Stuart
PA Roussel-UCLAF, Fr.
SO Eur. Pat. Appl., 55 pp.
CODEN: EPXXDW
DT Patent
LA French
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 524041	A2	19930120	EP 1992-401763	19920624
	EP 524041	A3	19940406		
	EP 524041	B1	19950920		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, PT, SE

US 5270343	A	19931214	GB 1991-13624	19910625
			US 1992-898135	19920615
CA 2072054	AA	19921226	GB 1991-13624	19910625
			CA 1992-2072054	19920623
ZA 9204664	A	19930628	GB 1991-13624	19910625
			ZA 1992-4664	19920624
JP 05294912	A2	19931109	GB 1991-13624	19910625
			JP 1992-188931	19920624
AT 128117	E	19951015	GB 1991-13624	19910625
			AT 1992-401763	19920624
ES 2077375	T3	19951116	GB 1991-13624	19910625
			ES 1992-401763	19920624
RU 2078076	C1	19970427	GB 1991-13624	19910625
			RU 1992-5052350	19920624
AU 9218531	A1	19930107	GB 1991-13624	19910625
AU 651217	B2	19940714	AU 1992-18531	19920625
BR 9202403	A	19930126	GB 1991-13624	19910625
			BR 1992-2403	19920625
CN 1073674	A	19930630	GB 1991-13624	19910625
			CN 1992-108833	19920625
HU 63938	A2	19931129	GB 1991-13624	19910625
HU 213030	B	19970128	HU 1992-2122	19920625
US 5459149	A	19951017	GB 1991-13624	19910625
			US 1994-309430	19940920
			GB 1991-13624	19910625
			US 1992-898135	19920615
			US 1993-99146	19930729

OS MARPAT 119:203161
GI



AB Title compds. Q(CH₂)_a(O)_bQ₁CR₂:CR₃CR₄:CR₅CXNR₁R_x [I; Q = mono- or bicyclic aromatic, dihalovinyl, R₆C.tplbond.C (R₆ = C1-4 alkyl, tri-C1-4-alkylsilyl, halo, H); Q₁ = 1,2-substituted cyclopropyl, substituted with C1-3 alkyl, C1-3 haloalkyl, C2-3 alkynyl, and -CN when Q₁ = (CH₂)₇; a = 0, 1; b = 0, 1; R₂-R₅ = identical or different with at least one being H, the others being H, halo, C1-4 alkyl, C1-4 haloalkyl; X = O, S; R₁ = (un)substituted Ph with various organic and inorg. groups; R_x = H, C1-8 alkyl or substituted PhCH₂], e.g., II, are prepared Compds. I or their salts are claimed for a variety of pesticidal activities, including arthropodocides, nematocides, molluscicides, and acaricides. Use of compds. I in surgical or therapeutic applications in humans and in animals (e.g., as parasiticides) is also claimed.

=> file reg
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION

FULL ESTIMATED COST

6.51 267.37

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL

CA SUBSCRIBER PRICE

ENTRY SESSION
-0.70 -4.90

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STRUCTURE FILE UPDATES: 17 NOV 2004 HIGHEST RN 783276-57-3
DICTIONARY FILE UPDATES: 17 NOV 2004 HIGHEST RN 783276-57-3

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> e 2,4-Pentadienoic acid, 5-phenoxy-/cn

E1	1	2,4-PENTADIENOIC ACID, 5-P-TOLYL-, ETHYL ESTER, (E,E)-/CN
E2	1	2,4-PENTADIENOIC ACID, 5-P-TOLYL-, METHYL ESTER/CN
E3	1 -->	2,4-PENTADIENOIC ACID, 5-PHENOXO-/CN
E4	1	2,4-PENTADIENOIC ACID, 5-PHENOXO-, ETHYL ESTER/CN
E5	1	2,4-PENTADIENOIC ACID, 5-PHENOXO-, METHYL ESTER/CN
E6	2	2,4-PENTADIENOIC ACID, 5-PHENYL-/CN
E7	1	2,4-PENTADIENOIC ACID, 5-PHENYL-, ((2-METHYL-1-OXO-2-PROPENYL)OXY)METHYL ESTER/CN
E8	1	2,4-PENTADIENOIC ACID, 5-PHENYL-, ((2-METHYL-1-OXO-2-PROPENYL)OXY)METHYL ESTER, POLYMER WITH BUTYL 2-METHYL-2-PROPENOATE AND 2-METHYL-2-PROPENOIC ACID/CN
E9	1	2,4-PENTADIENOIC ACID, 5-PHENYL-, (2,4,6-TRIOXO-1,3,5-TRIAZINE-1,3,5(2H,4H,6H)-TRIYL)TRI-2,1-ETHANEDIYL ESTER/CN
E10	1	2,4-PENTADIENOIC ACID, 5-PHENYL-, (2,4-DICHLOROPHENYL) (DIETHOXYPHOSPHINYL)METHYL ESTER, (2E,4E)-/CN
E11	1	2,4-PENTADIENOIC ACID, 5-PHENYL-, (2-CHLOROPHENYL) (DIETHOXYPHOSPHINYL)METHYL ESTER, (2E,4E)-/CN
E12	1	2,4-PENTADIENOIC ACID, 5-PHENYL-, (2E,4E)-/CN

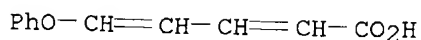
=> e3

L26 1 "2,4-PENTADIENOIC ACID, 5-PHENOXO-"/CN

=> d 126

L26 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
RN 17629-31-1 REGISTRY
CN **2,4-Pentadienoic acid, 5-phenoxy- (8CI, 9CI)** (CA INDEX NAME)
FS 3D CONCORD
MF C11 H10 O3
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)
DT.CA Caplus document type: Journal; Patent

RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)
RL.NP Roles from non-patents: PREP (Preparation)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
6.62	273.99

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-4.90

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FILE COVERS 1907 - 19 Nov 2004 VOL 141 ISS 21
FILE LAST UPDATED: 17 Nov 2004 (20041117/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> e 2,4-Pentadienoic acid, 5-phenoxy-/cn

REGISTRY INITIATED

Substance data EXPAND from CAS REGISTRY in progress...

E1	1	2,4-PENTADIENOIC ACID, 5-P-TOLYL-, ETHYL ESTER, (E,E)-/CN
E2	1	2,4-PENTADIENOIC ACID, 5-P-TOLYL-, METHYL ESTER/CN
E3	1 -->	2,4-PENTADIENOIC ACID, 5-PHENOXY-/CN
E4	1	2,4-PENTADIENOIC ACID, 5-PHENOXY-, ETHYL ESTER/CN
E5	1	2,4-PENTADIENOIC ACID, 5-PHENOXY-, METHYL ESTER/CN
E6	2	2,4-PENTADIENOIC ACID, 5-PHENYL-/CN
E7	1	2,4-PENTADIENOIC ACID, 5-PHENYL-, ((2-METHYL-1-OXO-2-PROPENYL)OXY)METHYL ESTER/CN
E8	1	2,4-PENTADIENOIC ACID, 5-PHENYL-, ((2-METHYL-1-OXO-2-PROPENYL

E9 1 L(OXY)METHYL ESTER, POLYMER WITH BUTYL 2-METHYL-2-PROPENOATE AND 2-METHYL-2-PROPENOIC ACID/CN
 E10 1 2,4-PENTADIENOIC ACID, 5-PHENYL-, (2,4,6-TRIOXO-1,3,5-TRIAZINE-1,3,5(2H,4H,6H)-TRIYL)TRI-2,1-ETHANEDIYL ESTER/CN
 E11 1 2,4-PENTADIENOIC ACID, 5-PHENYL-, (2,4-DICHLOROPHENYL) (DIETHOXYPHOSPHINYLMETHYL ESTER, (2E,4E)-/CN
 E12 1 2,4-PENTADIENOIC ACID, 5-PHENYL-, (2-CHLOROPHENYL) (DIETHOXYPHOSPHINYLMETHYL ESTER, (2E,4E)-/CN

=> 126

L27 3 L26

=> d 127 1-3 ti fbib abs

L27 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN
 TI Histone deacetylase inhibitors based on alphachalcogenmethylcarbonyl compounds
 AN 2003:950999 CAPLUS
 DN 140:4783
 TI Histone deacetylase inhibitors based on alphachalcogenmethylcarbonyl compounds
 IN Lan-Hargest, Hsuan-Yin; Kaufman, Robert J.
 PA Beacon Laboratories, Inc., USA
 SO PCT Int. Appl., 34 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2003099789	A1	20031204	WO 2003-US15838	20030521
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004023944	A1	20040205	US 2002-382077P	P 20020522
			US 2003-442191	20030521
			US 2002-382077P	P 20020522

OS MARPAT 140:4783

AB A compound having the formula AY1LY2C:X1CH2X2 with histone deacetylase inhibition activity is prepared wherein A is a cyclic moiety from cycloalkyl, cycloalkenyl, aryl etc.; each of Y1 and Y2 is -CH2-, -O-, -S-, -N(Rc) (Rc is hydrogen, alkyl, alkenyl, alkynyl, alkoxy, hydroxyalkyl, hydroxyl, or haloalkyl) etc.; L is a straight C3-12 chain containing ≥1 double bond and/or ≥1 triple bond; X1 is O or S; and X2 is -OR1, -SR1, or -SeR1, wherein R1 is hydrogen, alkyl, acyl, aryl or aralkyl. Thus, 12 mL of benzylacetone in 100 mL THF was treated with 18.3 mL chlorotrimethylsilane to give 18.1 g 2-((trimethylsilyl)oxy)-4-phenylbut-1-ene, which (8.8 g) was treated with m-chloroperbenzoic acid to give an enol ether epoxide, which was hydrolyzed to give 1-hydroxy-4-phenyl-2-butanone, which was treated with thionyl chloride to give 1-chloro-4-phenyl-2-butanone (.apprx.0.44 g), which was treated with 0.2 mL thioacetic acid to give S-(2-oxo-4-phenyl)butyl thioacetate in 91% purity.

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN
TI Histone deacetylase inhibitors based on trihalomethylcarbonyl compounds
AN 2003:950971 CAPLUS
DN 139:395619
TI Histone deacetylase inhibitors based on trihalomethylcarbonyl compounds
IN Lan-Hargest, Hsuan-Yin; Kaufman, Robert J.
PA Beacon Laboratories, Inc., USA
SO PCT Int. Appl., 26 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003099760	A1	20031204	WO 2003-US15996	20030521
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 2004029903	A1	20040212	US 2002-382075P	P 20020522
				US 2003-442175	20030521
				US 2002-382075P	P 20020522

OS MARPAT 139:395619
AB A compound having the formula $AY_1LY_2C:X_1CX_2$ with histone deacetylase inhibition activity is prepared wherein A is cyclic moiety from cycloalkyl, cycloalkenyl, or aryl etc.; each Y_1 and Y_2 is -O-, -S-, -N(Rc)-C(O)-O- (Rc is hydrogen, alkyl, alkenyl, alkynyl etc.); L is a straight C3-12 chain containing ≥ 1 double bond and/or ≥ 1 triple bond; X_1 is O or S; X_2 is a halogen. Thus, 65.0 g crotonaldehyde was treated with 927 mL of 1M solution of PhMgBr in THF to give 135.88 g 1-phenyl-2-buten-1-ol, which was treated with 2.3 mL concentrated HCl in 2750 mL water at room temperature to give 4-phenyl-3-buten-2-ol, which was treated with 14 mL DMF and 8.2 mL $POCl_3$ to give 8.78 g 5-phenyl-2,4-pentadienal, which was treated with an equal amount of acetic acid and piperidine followed by addition of 1,1,1-trifluoroacetone at room temperature to give 1,1,1-trifluoro-8-phenyl-3,5,7-octatrien-2-one.

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN
TI Preparation of phenoxy radicals
AN 1967:516385 CAPLUS
DN 67:116385
TI Preparation of phenoxy radicals
AU Horspool, William M.; Pauson, Peter L.
CS Univ. Strathclyde, Glasgow, UK
SO Monatshefte fuer Chemie (1967), 98(4), 1256-61
CODEN: MOCHAP
DT Journal
LA German
AB The decomposition of β -aryloxypropionyl peroxides was studied. Thus, $(PhOCH_2CH_2CO_2)_2$ decomposed at its m.p. or in boiling C_6H_{12} to $(PhOCH_2CH_2)_2$

or phenetole, resp., without elimination of C₂H₄. Similarly, 1,4-dihydro-4-phenoxynaphthoic acid could not be synthesized, but an elimination reaction was observed on treating dehydrobenzene with PhOCH:CHCH:CHCO₂Et (I), to give Et 1-naphthoate and PhOH. Treatment of I with MeO₂CC.tplbond.CCO₂Me gave the hemimellitic ester and PhOH, while with maleic anhydride normal addition to the phenoxycyclohexene derivative was observed.

=> file reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
13.37	288.22

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-2.10	-7.00

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FILE 'REGISTRY' ENTERED AT 08:00:53 ON 19 NOV 2004
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STRUCTURE FILE UPDATES: 17 NOV 2004 HIGHEST RN 783276-57-3
DICTIONARY FILE UPDATES: 17 NOV 2004 HIGHEST RN 783276-57-3

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> e 1-Cyclohexene-1-sorbic acid, γ,2,6,6-tetramethyl-/cn

E1	1	1-CYCLOHEXENE-1-SORBALDEHYDE, 4-METHOXY-Γ,2,6,6-TETRAMETHYL-/CN
E2	1	1-CYCLOHEXENE-1-SORBALDEHYDE, 6-ISOBUTYL-Γ,2,6-TRIMETHYL-/CN
E3	1 -->	1-CYCLOHEXENE-1-SORBIC ACID, Γ,2,6,6-TETRAMETHYL-/CN
E4	1	1-CYCLOHEXENE-1-SORBIC ACID, Γ,2,6,6-TETRAMETHYL-, ETHYL ESTER/CN
E5	1	1-CYCLOHEXENE-1-SORBIC ACID, Γ,2,6,6-TETRAMETHYL-, METHYL ESTER/CN
E6	1	1-CYCLOHEXENE-1-SUCCINIC ACID/CN
E7	1	1-CYCLOHEXENE-1-SUCCINIC ACID, A-CYANO-6-METHYL-, DIETHYL ESTER/CN
E8	1	1-CYCLOHEXENE-1-SUCCINIC ACID, A-METHYL ESTER/CN
E9	1	1-CYCLOHEXENE-1-SUCCINIC ACID, B-METHYL-/CN
E10	1	1-CYCLOHEXENE-1-SUCCINIC ACID, B-METHYL-, A-METHYL ESTER/CN
E11	1	1-CYCLOHEXENE-1-SUCCINIC ACID, 1-ETHYL ESTER/CN
E12	1	1-CYCLOHEXENE-1-SUCCINIC ACID, 2-METHYL-/CN

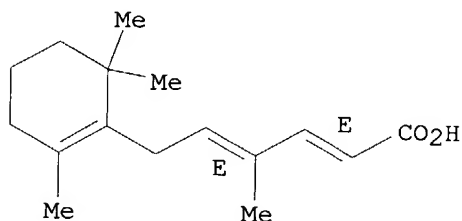
=> e3

L28 1 "1-CYCLOHEXENE-1-SORBIC ACID, γ ,2,6,6-TETRAMETHYL-"/CN

=> d 128

L28 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
RN 110252-16-9 REGISTRY
CN 1-Cyclohexene-1-sorbic acid, γ ,2,6,6-tetramethyl- (6CI)
(CA INDEX NAME)
FS STEREOSEARCH
MF C16 H24 O2
SR CAOLD
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS
(*File contains numerically searchable property data)
DT.CA Caplus document type: Journal; Patent
RL.P Roles from patents: NORL (No role in record)
RL.NP Roles from non-patents: NORL (No role in record)

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE)
5 REFERENCES IN FILE CAPLUS (1907 TO DATE)
3 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
6.62	294.84

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-7.00

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=> 128

L29 5 L28

=> 128/prep

5 L28

3224633 PREP/RL

L30 0 L28/PREP

(L28 (L) PREP/RL)

=> d 129 1-3 ti fbib abs

L29 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN
TI α,β -Unsaturated carboxylic acids and their esters
AN 1959:99382 CAPLUS
DN 53:99382

OREF 53:17880a-e

TI α,β -Unsaturated carboxylic acids and their esters

IN Isler, Otto; Ruegg, Rudolf

PA F. Hoffmann-La Roche & Co. Akt.-Ges.

DT Patent

LA Unavailable

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 949886		19560927	DE	
AB	ClCH:CHOEt (I) reacts in liquid NH ₃ with 2 equivs. NaNH ₂ or LiNH ₂ to give Na(or K)C.tplbond.COEt which is condensed in the same medium with aldehydes or ketones at a ratio of 1:1 for mono- and 2:1 for dialdehydes and diketones. Hydrolysis with NH ₄ Cl and isomerization of the ethynylcarbinol formed yields the α,β -unsatd. carboxylic ester. If the aldehydes or ketones used contain free OH or CO ₂ H groups, addnl. equivs. of NaNH ₂ or LiNH ₂ are required for each functional group. To a solution of NaNH ₂ in NH ₃ 37.5 g. I is added while stirring and after 10 min. dropwise 31 g. 6-methyl-5-hepten-2-one (II). The mixture is stirred 40 hrs., 45 g. NH ₄ Cl added and the NH ₃ evaporated. After addition of 800 cc. ligroine, filtration and evaporation, distillation of the residue yields 10 g. II and 26 g. 1-ethoxy-3-hydroxy-3,7-dimethyl-6-octen-1-yne, b0.05 80°; its solution in 300 cc. Et ₂ O is shaken 16 hrs. with 100 cc. 10% H ₂ SO ₄ , diluted with H ₂ O and the Et ₂ O layer worked up to yield 21 g. 3,7-dimethyl-2,6-octadienoic acid (III) Et ester which is hydrolyzed with 12.5 g. NaOH and 35 cc. H ₂ O in 350 cc. MeOH to yield 16 g. III, b0.03 90°, n _D 23D 1.4769. Similarly are prepared: 6-(2,6,6-trimethyl-1-cyclohexen-1-yl)-4-methyl-2,4-hexadienoic acid (IV), λ 255 m μ , E1%1cm. 617 (EtOH) [Me ester b0.07 116°, n _D 21D 1.5242, λ 268 m μ , E1%1cm. 608 (EtOH)]; cinnamic acid, m. 125-6°; 2,6,6-trimethyl-2-cyclohexen-1-ylideneacetic acid, m. 53-5° (ligroine), λ 252.5 m μ , E1%1cm. 575 (EtOH); 2-pentenoic acid b10 94°, m. -2°, n _D 22.5D 1.4382, λ 212.5 m μ , E1%1cm. 750 (EtOH), 3-methyl-2-pentenoic acid, b10 99-102°, n _D 22D 1.4556, λ 218 m μ , E1%1cm. 860 (EtOH); β -methylcinnamic acid, b0.05 105-8°, λ 251.5 m μ , E1%1cm. 503 (EtOH); 5,17(20)-pregnadien-3 β -ol-21-oic acid, m. 244°, λ 221 m μ , E1%1cm. 330 (EtOH).				

L29 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN
 TI Continuous process for the oxidation of hydrocarbons
 AN 1958:103859 CAPLUS
 DN 52:103859
 OREF 52:18218d-e
 TI Continuous process for the oxidation of hydrocarbons
 IN Tsykskovskii, V. K.; Shcheglova, Ts. N.; Pylaeva, T. I.; Meshchaninov, S. M.; Soltan, S. G.
 DT Patent
 LA Unavailable
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	SU 109712		19580527	SU	
AB	Hydrocarbons are oxidized to carboxylic acids; the acids formed are removed from the cycle and saponified with NaOH in an impeller type mixer. The Na soaps are removed by centrifuging and the unreacted hydrocarbons are returned to the cycle together with fresh hydrocarbons in a volume corresponding to the quantity of soap removed.				

L29 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN
 TI α,β -Unsaturated carboxylic acids and their esters
 AN 1958:103858 CAPLUS
 DN 52:103858
 OREF 52:18218c-d
 TI α,β -Unsaturated carboxylic acids and their esters
 IN Isler, Otto; Ruegg, Rudolf
 PA Hoffmann-La Roche Inc.
 DT Patent
 LA Unavailable
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2849466		19580826	US	
AB	See Brit. 772,199 (C.A. 52, 1223g).				

=> logoff hold

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
11.23	306.07

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-2.10	-9.10

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SESSION WILL BE HELD FOR 60 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 08:03:58 ON 19 NOV 2004

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LOGINID:SSSPTA1623PAZ

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
 SESSION RESUMED IN FILE 'CAPLUS' AT 08:31:47 ON 19 NOV 2004
 FILE 'CAPLUS' ENTERED AT 08:31:47 ON 19 NOV 2004

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	11.23	306.07

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.10	-9.10

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	12.11	306.95

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.10	-9.10

FILE 'REGISTRY' ENTERED AT 08:32:50 ON 19 NOV 2004
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STRUCTURE FILE UPDATES: 17 NOV 2004 HIGHEST RN 783276-57-3
DICTIONARY FILE UPDATES: 17 NOV 2004 HIGHEST RN 783276-57-3

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

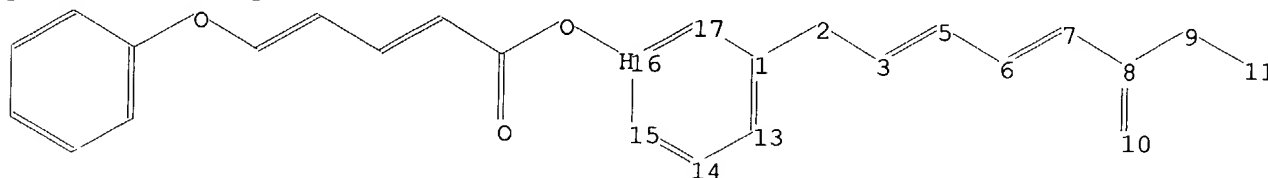
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Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\Examination Auxillary files\10025947\10025947 RCE rphenoxy pentadienoic.str



chain nodes :

2 3 5 6 7 8 9 10 11

ring nodes :

1 13 14 15 16 17

chain bonds :

1-2 2-3 3-5 5-6 6-7 7-8 8-9 8-10 9-11

ring bonds :

1-13 1-17 13-14 14-15 15-16 16-17

exact/norm bonds :

1-2 2-3
 exact bonds :
 3-5 5-6 6-7 7-8 9-11
 normalized bonds :
 1-13 1-17 8-9 8-10 13-14 14-15 15-16 16-17

G1:S,N,O

Match level :

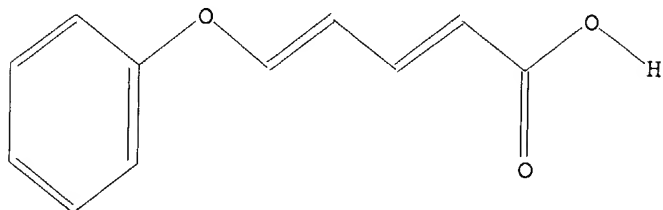
1:Atom 2:CLASS 3:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS
 11:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom

L31 STRUCTURE UPLOADED

=> d 131

L31 HAS NO ANSWERS

L31 STR



G1 S,N,O

Structure attributes must be viewed using STN Express query preparation.

=> search 131 sss sam

SAMPLE SEARCH INITIATED 08:33:14 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 46 TO ITERATE

100.0% PROCESSED 46 ITERATIONS

SEARCH TIME: 00.00.01

1 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 514 TO 1326

PROJECTED ANSWERS: 1 TO 80

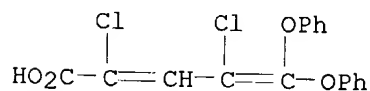
L32 1 SEA SSS SAM L31

=> d scan

L32 1 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN 2,4-Pentadienoic acid, 2,4-dichloro-5-oxo-, diphenyl acetal (8CI)

MF C17 H12 Cl2 O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> search l31 sss full

FULL SEARCH INITIATED 08:33:29 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 601 TO ITERATE

100.0% PROCESSED 601 ITERATIONS

SEARCH TIME: 00.00.01

5 ANSWERS

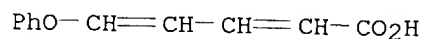
L33 5 SEA SSS FUL L31

=> d scan

L33 5 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN 2,4-Pentadienoic acid, 5-phenoxy- (8CI, 9CI)

MF C11 H10 O3



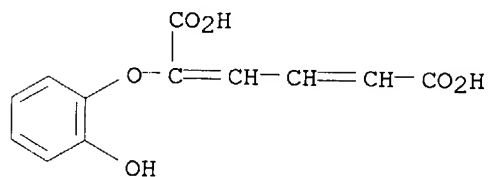
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):5

L33 5 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN 2,4-Hexadienedioic acid, 2-(2-hydroxyphenoxy)- (9CI)

MF C12 H10 O6

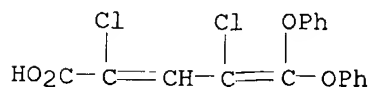


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L33 5 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

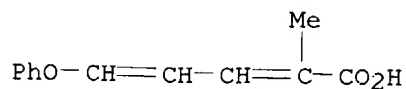
IN 2,4-Pentadienoic acid, 2,4-dichloro-5-oxo-, diphenyl acetal (8CI)

MF C17 H12 Cl2 O4



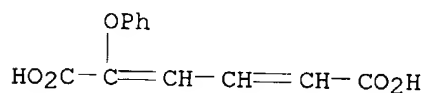
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L33 5 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2,4-Pentadienoic acid, 2-methyl-5-phenoxy- (8CI)
MF C12 H12 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L33 5 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2,4-Hexadienedioic acid, 2-phenoxy- (9CI)
MF C12 H10 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> logoff hold

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
156.68	463.63

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-9.10

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NEWS 3 JUL 12 BEILSTEIN enhanced with new display and select options,
resulting in a closer connection to BABS
NEWS 4 AUG 02 IFIPAT/IFIUDB/IFICDB reloaded with new search and display
fields
NEWS 5 AUG 02 CAlus and CA patent records enhanced with European and Japan
Patent Office Classifications
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NEWS 7 AUG 27 BIOCOMMERCE: Changes and enhancements to content coverage
NEWS 8 AUG 27 BIOTECHABS/BIOTECHDS: Two new display fields added for legal
status data from INPADOC
NEWS 9 SEP 01 INPADOC: New family current-awareness alert (SDI) available
NEWS 10 SEP 01 New pricing for the Save Answers for SciFinder Wizard within
STN Express with Discover!
NEWS 11 SEP 01 New display format, HITSTR, available in WPIDS/WPINDEX/WPIX
NEWS 12 SEP 27 STANDARDS will no longer be available on STN
NEWS 13 SEP 27 SWETSCAN will no longer be available on STN
NEWS 14 OCT 28 KOREAPAT now available on STN
NEWS 15 NOV 18 Current-awareness alerts, saved answer sets, and current
search transcripts to be affected by CERAB, COMPUAB, ELCOM,
and SOLIDSTATE reloads

NEWS EXPRESS OCTOBER 29 CURRENT WINDOWS VERSION IS V7.01A, CURRENT
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
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FILE 'HOME' ENTERED AT 10:43:21 ON 19 NOV 2004

=> file reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.42	0.42

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 10:44:13 ON 19 NOV 2004

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STRUCTURE FILE UPDATES: 17 NOV 2004 HIGHEST RN 783276-57-3
DICTIONARY FILE UPDATES: 17 NOV 2004 HIGHEST RN 783276-57-3

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

```
=> e 7,7-diphenyl-2,4,6-heptatrienoic acid/cn
E1      1      7,7-DINORYUEHCHUKENE/CN
E2      1      7,7-DIOCTYL-7-STANNA-2,6,8-TRIOXASPIRO(3.5)NONANE/CN
E3      0 --> 7,7-DIPHENYL-2,4,6-HEPTATRIENOIC ACID/CN
E4      1      7,7-DIPHENYL-6-HEPTENE-2,5-DIONE/CN
E5      1      7,7-DIPHENYL-6-OXABICYCLO(3.2.0)HEPT-1-ENE/CN
E6      1      7,7-DIPHENYL-7H-BENZO(2,3-G)CHROMENE/CN
E7      1      7,7-DIPHENYLBICYCLO(3.2.0)HEPT-2-EN-6-ONE/CN
E8      1      7,7-DIPHENYLBICYCLO(3.2.0)HEPTAN-6-ONE/CN
E9      1      7,7-DIPHENYLDIHYDROMORPHINONE/CN
E10     1      7,7-DIPHENYLDIHYDROMORPHINONE HYDROCHLORIDE/CN
E11     1      7,7-DIPHENYLHEPT-6-ENOIC ACID/CN
E12     1      7,7-DIPHENYLHEPTA-4,6-DIENOIC ACID/CN
```

=> e12

L1 1 "7,7-DIPHENYLHEPTA-4,6-DIENOIC ACID"/CN

=> d l1

```
L1      ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2004 ACS on STN
RN      134613-72-2  REGISTRY
CN      4,6-Heptadienoic acid, 7,7-diphenyl- (9CI)  (CA INDEX NAME)
OTHER NAMES:
CN      7,7-Diphenylhepta-4,6-dienoic acid
FS      3D CONCORD
MF      C19 H18 O2
SR      CA
LC      STN Files:  CA, CAPLUS
DT.CA   Caplus document type:  Journal
RL.NP   Roles from non-patents:  PREP (Preparation); RACT (Reactant or reagent)
```

$\text{Ph}_2\text{C}=\text{CH}-\text{CH}=\text{CH}-\text{CH}_2-\text{CH}_2-\text{CO}_2\text{H}$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus

COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
7.46	7.88

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FILE COVERS 1907 - 19 Nov 2004 VOL 141 ISS 22
FILE LAST UPDATED: 18 Nov 2004 (20041118/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> l1

L2 1 L1

=> d l2 ti fbib abs

L2 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN
TI Photocycloeliminations of bicyclic cyclobutanones. I. Solvent effects on distribution of products
AN 1991:448482 CAPLUS
DN 115:48482
TI Photocycloeliminations of bicyclic cyclobutanones. I. Solvent effects on distribution of products
AU Lee-Ruff, E.; Hayes, I. E. E.; Kazarians-Moghaddam, H.
CS Dep. Chem., York Univ., Toronto, ON, M3J 1P3, Can.
SO Structural Chemistry (1991), 2(2), 175-83
CODEN: STCHES; ISSN: 1040-0400
DT Journal
LA English
OS CASREACT 115:48482
AB The extent of photocycloelimination in α -arylcyclobutanones can be controlled by solvent effects indicative of reversible oxacarbene formation. Substituent effects at C-3 as well as ring size of the adjacent fused ring play important roles in these reactions. The efficient photocycloelimination of such bicyclic ketones in nonpolar aprotic solvents constitutes a route to terminally unsatd. esters in an overall two-step metathesis reaction the mechanism of which is discussed.

=> d l2 it

L2 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN
IT Carboxylic acids, preparation
RL: PREP (Preparation)
(2-step metathesis reaction involving bicyclic cyclobutanones as route to)
IT Double decomposition
(as stereospecific road to unsatd. esters, mechanism and solvent effects on)

IT Solvent effect
Substituent effect
(on photocycloelimination of bicyclic cyclobutanones)

IT Ring cleavage
(photochem., of bicyclic cyclobutanones, solvent effect and mechanism of)

IT Carboxylic acids, esters
RL: PREP (Preparation)
(unsatd., esters, 2-step metathesis reaction involving bicyclic cyclobutanones as route to)

IT 67093-47-4, 8,8-Diphenylbicyclo[4.2.0]oct-2-en-7-one
RL: PRP (Properties)
(hydrogenation and photocycloelimination of)

IT 64-17-5, Ethanol, uses and miscellaneous 67-56-1, Methanol, uses and miscellaneous
RL: USES (Uses)
(photolysis of bicyclocyclobutanones in presence of, unsatd. esters by)

IT 94385-09-8, 7,7-Diphenylheptanoic acid
RL: PRP (Properties)
(photolysis of bicyclocyclobutanones in presence of, unsatd. esters by)

IT 87274-24-6P **134613-72-2P**, 7,7-Diphenylhepta-4,6-dienoic acid 134613-92-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenation of)

IT 134613-71-1P 134613-90-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

IT 4173-55-1P, 8,8-Diphenylbicyclo[4.2.0]octan-7-one 87274-16-6P, 7,7-Diphenylbicyclo[3.2.0]heptan-6-one
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and photocycloelimination of)

IT 87274-22-4P, Methyl 8,8-diphenyl-7-octenoate 122213-92-7P, 7,7-Diphenylhept-6-enoic acid 134613-70-0P 134613-73-3P, Ethyl 8,8-diphenyloctanoate 134613-74-4P 134613-91-5P 134613-93-7P 134679-05-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 5452-28-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, hydrogenation, and photocycloelimination of)

IT 87274-21-3P, Methyl 7,7-diphenylhept-6-enoate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, saponification, and hydrogenation of)

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
5.06	12.94

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-0.70	-0.70

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FILE 'CAPLUS' ENTERED AT 10:48:44 ON 19 NOV 2004

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FILE COVERS 1907 - 19 Nov 2004 VOL 141 ISS 22
FILE LAST UPDATED: 18 Nov 2004 (20041118/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> file reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.44	13.38

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-0.70

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 17 NOV 2004 HIGHEST RN 783276-57-3
DICTIONARY FILE UPDATES: 17 NOV 2004 HIGHEST RN 783276-57-3

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> e 5,5-diphenyl-2,4-pentadienoic acid/cn

E1	1	5,5-DIPHENYL-2,4-IMIDAZOLIDINEDIONE/CN
E2	1	5,5-DIPHENYL-2,4-PENTADIENAL/CN
E3	0 -->	5,5-DIPHENYL-2,4-PENTADIENOIC ACID/CN
E4	1	5,5-DIPHENYL-2,4-PENTADIENYLIDENE-4,4'-BIS(N,N-DIETHYL-M-TOLUIDINE)/CN
E5	1	5,5-DIPHENYL-2,5-DIHYDRO-2-FURANONE/CN
E6	1	5,5-DIPHENYL-2-(2'-PIPERIDINOETHYL)-1,3-DIOXOLAN-4-ONE/CN
E7	1	5,5-DIPHENYL-2-(2'-PIPERIDINOETHYL)-1,3-DIOXOLAN-4-ONE HYDROCHLORIDE/CN
E8	1	5,5-DIPHENYL-2-(2'-PIPERIDINOETHYL)-1,3-DIOXOLAN-4-ONE HYDROCHLORIDE/CN

E9	1	HLORIDE/CN
E10	1	5,5-DIPHENYL-2-(P-TOLYLTHIOCARBAMOYL) GLYCOCYAMIDINE/CN
E11	1	5,5-DIPHENYL-2-(PHENYLTHIOCARBAMOYL) GLYCOCYAMIDINE/CN
E12	1	5,5-DIPHENYL-2-CYCLOPENTENE/CN
		5,5-DIPHENYL-2-ETHOXYOXAZOLIDIN-4-ONE/CN

=> logoff hold

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
1.68	15.06

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-0.70

CA SUBSCRIBER PRICE

SESSION WILL BE HELD FOR 60 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 10:51:31 ON 19 NOV 2004

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

***** RECONNECTED TO STN INTERNATIONAL *****
 SESSION RESUMED IN FILE 'REGISTRY' AT 10:54:10 ON 19 NOV 2004
 FILE 'REGISTRY' ENTERED AT 10:54:10 ON 19 NOV 2004
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COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
1.68	15.06

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-0.70

CA SUBSCRIBER PRICE

=> e 2-Pentenedioic acid, 4-(((2-(methoxycarbonyl)phenyl)amino)methylene)-, 5-methyl ester, (? ,Z)-/cn

E1	1	2-PENTENEDIOIC ACID, 4-(((2-(2-ETHOXY-2-OXOETHYL) PHENYL) AMINO) METHYLENE)-, 5-METHYL ESTER, (? ,Z)-/CN
E2	1	2-PENTENEDIOIC ACID, 4-(((2-(ACETYLAMINO)-1,1-DIMETHYLETHYL) METHYLAMINO) METHYLENE)-, DIETHYL ESTER, (E,E)-/CN
E3	0 -->	2-PENTENEDIOIC ACID, 4-(((2-(METHOXYCARBONYL) PHENYL) AMINO) ME THYLENE)-, 5-METHYL ESTER, (? ,Z)-/CN
E4	1	2-PENTENEDIOIC ACID, 4-(((2-(METHOXYCARBONYL) PHENYL) AMINO) ME THYLENE)-, 5-METHYL ESTER, (2E,4E)-/CN
E5	1	2-PENTENEDIOIC ACID, 4-(((2-(METHOXYCARBONYL) PHENYL) AMINO) ME THYLENE)-, 5-METHYL ESTER, (? ,Z)-/CN
E6	1	2-PENTENEDIOIC ACID, 4-(((2-AMINOPHENYL) AMINO) METHYLENE)-, 5-METHYL ESTER, (Z,Z)-/CN
E7	1	2-PENTENEDIOIC ACID, 4-(((2-CHLOROPHENYL) AMINO) METHYLENE)-, 5-METHYL ESTER, (2E,4E)-/CN
E8	1	2-PENTENEDIOIC ACID, 4-(((2-CHLOROPHENYL) AMINO) METHYLENE)-, 5-METHYL ESTER, (? ,Z)-/CN
E9	1	2-PENTENEDIOIC ACID, 4-(((2-HYDROXY-1-PHENYLETHYL) AMINO) METH YLENE)-, DIMETHYL ESTER/CN
E10	1	2-PENTENEDIOIC ACID, 4-(((2-METHOXY-2-OXOETHYL) AMINO) METHYLE

E11 1 NE)-, DIETHYL ESTER, (2E,4Z)-/CN
 2-PENTENEDIOIC ACID, 4-(((2-METHOXYPHENYL)AMINO)METHYLENE)-,
 DIETHYL ESTER, (2E,4Z)-/CN
 E12 1 2-PENTENEDIOIC ACID, 4-(((3,4-DICHLOROPHENYL)AMINO)METHYLENE
)-, 5-METHYL ESTER/CN

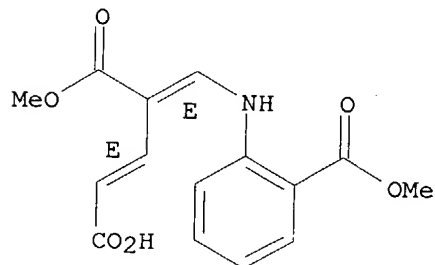
=> e4

L3 1 "2-PENTENEDIOIC ACID, 4-(((2-(METHOXYCARBONYL)PHENYL)AMINO)METHY
 LENE)-, 5-METHYL ESTER, (2E,4E)-"/CN

=> d 13

L3 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
 RN 344901-55-9 REGISTRY
 CN **2-Pentenedioic acid, 4-[[[2-(methoxycarbonyl)phenyl]amino]methylene]-
 , 5-methyl ester, (2E,4E)- (9CI) (CA INDEX NAME)**
 FS STEREOSEARCH
 MF C15 H15 N O6
 SR Reaction Database
 LC STN Files: CASREACT

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

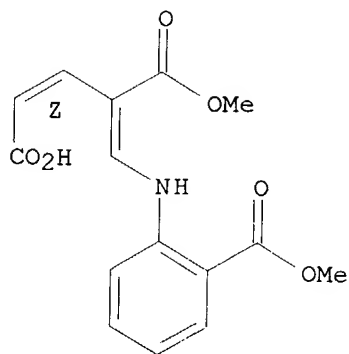
=> e5

L4 1 "2-PENTENEDIOIC ACID, 4-(((2-(METHOXYCARBONYL)PHENYL)AMINO)METHY
 LENE)-, 5-METHYL ESTER, (? ,Z)-"/CN

=> d 14

L4 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
 RN 89537-99-5 REGISTRY
 CN **2-Pentenedioic acid, 4-[[[2-(methoxycarbonyl)phenyl]amino]methylene]-
 , 5-methyl ester, (? ,Z)- (9CI) (CA INDEX NAME)**
 FS STEREOSEARCH
 MF C15 H15 N O6
 LC STN Files: CA, CAPLUS
 DT.CA Caplus document type: Journal
 RL.NP Roles from non-patents: PREP (Preparation)

Double bond geometry as described by E or Z.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
15.34	28.72

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-0.70

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FILE 'CAPLUS' ENTERED AT 10:56:07 ON 19 NOV 2004
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FILE COVERS 1907 - 19 Nov 2004 VOL 141 ISS 22
FILE LAST UPDATED: 18 Nov 2004 (20041118/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

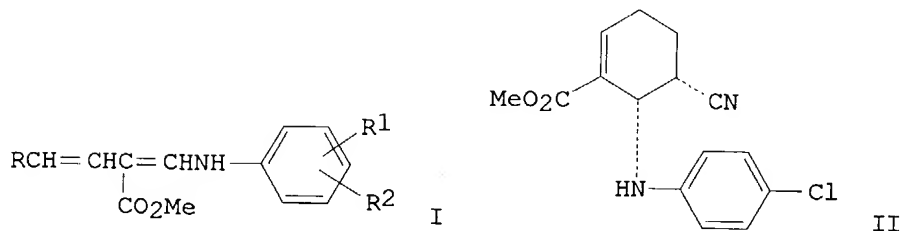
=> 14

L5 1 L4

=> d 15 ti fbib abs

L5 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN
TI Chemistry of coumalic acid derivatives. I. Synthesis and Diels-Alder reactions of 1-arylamino-2-(methoxycarbonyl)butadiene

AN 1984:156297 CAPLUS
 DN 100:156297
 TI Chemistry of coumalic acid derivatives. I. Synthesis and Diels-Alder reactions of 1-arylamino-2-(methoxycarbonyl)butadiene
 AU Kvita, Vratislav; Sauter, Hanspeter; Rihs, Grete
 CS Zent. Forschungslab., Ciba-Geigy A.-G., Basel, CH-4002, Switz.
 SO Helvetica Chimica Acta (1983), 66(8), 2769-77
 CODEN: HCACAV; ISSN: 0018-019X
 DT Journal
 LA German
 OS CASREACT 100:156297
 GI



AB The nucleophilic attack of $R_1R_2C_6H_3NH_2$ ($R_1 = 2-, 3-, 4-Cl, 3-F_3C, 3-O_2N, 4-MeO, 2-CO_2Me, 2-CH_2CO_2Et, R_2 = H$; $R_1 = 2-Me, 2-, 3-Cl, R_2 = Cl$; $R_1 = 3-Cl, R_2 = 5-Cl, R_1 = 3-MeO, R_2 = 4-MeO$) at position 6 of Me coumalate cleaved the α -pyrone ring to give butadienecarboxylic acids I ($R = CO_2H$). Some of these I were easily decarboxylated at room temperature in polar aprotic solvents to give the unisolated butadienes I ($R = H, R_1 = 3-, 4-Cl, 2-CO_2Me, 2-CH_2CO_2Et, R_2 = H, R_1 = 2-Me, 2-, 3-Cl, R_2 = 4-Cl$). These underwent smooth regio- and stereospecific Diels-Alder reactions with various dienophiles to give, e.g., II, the crystal structure of which is given.

=> logoff hold

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
3.87	32.59

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-0.70	-1.40

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SESSION WILL BE HELD FOR 60 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 10:58:12 ON 19 NOV 2004